



THEORY OF LARGE QUANTAL SYSTEMS  
AND THE  
QUANTUM THEORY OF MEASUREMENT

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## ABSTRACT

The consistency problem of quantum mechanics may be resolved by regarding any measurement performed on an atomic system as essentially involving an interaction between the atomic system and a macroscopic measuring apparatus and the subsequent behaviour of the apparatus in producing a signal to indicate the result of the measurement. Of central importance in such an approach, therefore, is the study of large quantal systems.

Along these lines, two approaches to the consistency problem have been provided; one, by the Italian group of Daneri, Loinger and Prosperi, based on a time-independent ergodic theory of large quantal systems; the other by the Belgian group of George, Prigogine and Rosenfeld, based on a time-dependent theory.

In this thesis these two theories are compared and are shown to be equivalent.

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## CONTENTS

	Page
1. INTRODUCTION .....	1
2. ERGODIC THEORY OF LARGE QUANTAL SYSTEMS .....	6
2.1 Macroscopic Observables .....	6
2.2 Ergodic Behaviour and Approach to Equilibrium .....	13
Ergodic Theory of the Italian Group .....	16
3. RESOLUTION OF THE MEASUREMENT PROBLEM BY THE APPROACH OF THE ITALIAN GROUP .....	23
3.1 Example of a Typical Measuring Process .....	23
3.2 General Theory of the Measuring Process .....	26
4. SUPERSPACE THEORY OF LARGE QUANTAL SYSTEMS .....	35
4.1 Basic Modes .....	35
4.2 Liouville Equation .....	36
4.3 Mathematical Preliminaries .....	40
Definitions .....	41
Projection Operators and Superoperators .....	45
4.4 Correlation and Vacuum of Correlations Subspaces .....	46
4.5 Reduced Properties .....	50
4.6 Outline of the Approach of the Belgian Group in the $\nu$ -N Notation .....	53
4.7 Superspace Approach .....	62
4.8 Heisenberg Picture and Time-reversal .....	69
4.9 The Projectors $\tilde{\Pi}$ and $\hat{\Pi}$ and Subdynamics .....	75
4.10 Invariants of the System .....	83
4.11 Condition of Dissipativity .....	92
4.12 Physical Interpretation of the Theory .....	92
Macroscopic Observations and Subdynamics .....	92
Non-dissipative Systems .....	94
Dissipative Systems .....	96
Summary and Further Points of Interpretation .....	99

	Page
5. RESOLUTION OF THE MEASUREMENT PROBLEM BY THE APPROACH OF THE BELGIAN GROUP .....	102
6. MODIFIED MACROSCOPIC DESCRIPTION .....	111
7. COMPARISON BETWEEN THE ERGODIC AND SUPERSPACE THEORIES .....	117
7.1 Macroscopic Description .....	117
7.2 Discussion of the Measuring Process on an Atomic System .....	118
7.3 Approach to Equilibrium .....	121
7.4 Concluding Remarks .....	124
REFERENCES .....	126

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## 1. INTRODUCTION

The measurement problem of quantum mechanics arises from the interpretation of the axioms of the theory concerning the measurement of a system of atomic dimensions.

The "Copenhagen interpretation"<sup>1)</sup> of quantum mechanics emphasizes the fact that the measurement problem arises from the necessity of using classical concepts in the laws governing individual atomic processes, since these are the concepts that are of direct experience to the human observer, and since any observation on an atomic system necessarily involves the use of a measuring apparatus of macroscopic dimensions. The description of an atomic process therefore cannot be separated from the experimental conditions of observation which includes the specification of the apparatus, which indicates the result of each measurement with a signal of macroscopic nature. It is precisely the production of the signal at the macroscopic level which makes it possible to describe the behaviour of the atomic system in terms of the familiar classical concepts.

It is to be stressed that this approach to the measurement problem maintains the objectivity of the physical description, thus ensuring its validity for all possible observers.

(This principle was not upheld in the approach of von Neumann (ref. <sup>2)</sup> chapters 5 and 6), in which the human observer is included in the dynamical system.)

In terms of this approach, the measurement problem of quantum mechanics reduces to a consistency problem which may

be summarized as follows:

Let the state of a system of atomic dimensions be given by the state vector  $|\phi(o)\rangle$  at time  $t = 0$  and let the observable of interest be represented by the operator  $A$ . Assume that the measurement is a maximal one. This implies that the spectrum of  $A$  is non-degenerate. Without loss of generality it may be assumed for convenience of notation that the spectrum of  $A$  is discrete. Let  $\{|\phi_r\rangle\}$  denote a complete orthogonal basis of eigenvectors of  $A$  for the Hilbert space of the atomic system and let  $a_r$  denote the eigenvalue of  $|\phi_r\rangle$ . Then  $|\phi(o)\rangle$  may be expanded in the form

$$|\phi(o)\rangle = \sum_r c_r |\phi_r\rangle \quad (1.1)$$

Let the observation of  $A$  be performed at time  $t = 0$ .

According to the measurement axiom of quantum mechanics, if the observation yields the result  $a_k$ , the state of the system immediately after the measurement is given by  $|\phi_k\rangle$  and the probability for the occurrence of this result is given by  $|c_k|^2$ . At a later time  $t$  the state of the system is given, on the basis of the Schrödinger equation, by

$$|\phi_k(t)\rangle = e^{-\frac{i}{\hbar} H t} |\phi_k\rangle \quad (1.2)$$

In density operator notation this situation can be represented more conveniently as follows:

Let  $\rho = |\phi\rangle\langle\phi|$  denote the density operator corresponding to the pure state  $|\phi\rangle$ . Then before the measurement



$$\rho(0) = |\phi(0)\rangle\langle\phi(0)| = \sum_{rr'} c_r c_{r'}^* |\phi_r\rangle\langle\phi_{r'}| \quad (1.3)$$

Denote by  $\rho_k(0)$  the density operator for the system for the case in which the result of the measurement was  $a_k$ .

$$\rho_k(0) = |\phi_k\rangle\langle\phi_k| \quad (1.4)$$

At a later time  $t$

$$\rho_k(t) = e^{-\frac{i}{\hbar} H t} |\phi_k\rangle\langle\phi_k| e^{\frac{i}{\hbar} H t} \quad (1.5)$$

On the basis of this information the probability of finding the system in the state  $|\chi\rangle$  at time  $t$  is given by

$$U_{|\chi\rangle}^k(t) = \text{tr}(\rho_k(t) P_{|\chi\rangle}) \quad (1.6)$$

where  $P_{|\chi\rangle}$  is the projection operator onto the state  $|\chi\rangle$ .

If the result of the measurement at time  $t = 0$  is not known by the observer, he will assign to the probability  $U_{|\chi\rangle}(t)$  the value

$$U_{|\chi\rangle}(t) = \sum_k |c_k|^2 U_{|\chi\rangle}^k(t) \quad (1.7)$$

on the basis of the addition law for probabilities. From eq. (6) this becomes

$$U_{|\chi\rangle}(t) = \sum_k |c_k|^2 \text{tr}(\rho_k(t) P_{|\chi\rangle}) = \text{tr}(\rho(t) P_{|\chi\rangle}) \quad (1.8)$$

where

$$\rho(t) = \sum_k |c_k|^2 \rho_k(t) = \sum_k |c_k|^2 e^{-\frac{i}{\hbar} H t} |\phi_k\rangle \langle \phi_k| e^{\frac{i}{\hbar} H t} \quad (1.9)$$

Eq. (9) therefore gives the density operator for the system at time  $t$  on the basis of the fact that the measurement at time  $t = 0$  was performed, but without the knowledge of the outcome of this measurement.

Now suppose that no measurement was performed at time  $t = 0$ . The density operator for the system at time  $t$  would then be given by

$$\rho(t) = |\phi(t)\rangle \langle \phi(t)| = \sum_{k, k'} c_k c_{k'}^* e^{-\frac{i}{\hbar} H t} |\phi_k\rangle \langle \phi_{k'}| e^{\frac{i}{\hbar} H t} \quad (1.10)$$

which differs from the density operator given by eq. (9) by the additional interference terms  $k \neq k'$ . In effect the measurement at time  $t = 0$  has resulted in the elimination of these interference terms - an irreversible change in the density operator which alters the predictions that may be made on the results of future measurements by an observer who knows that this initial measurement was performed but does not know the result of the measurement. This change in the "state" of the system is formally referred to as the reduction of the state vector of the system.

The consistency problem of quantum mechanics is whether it can be shown that the reduction of the state vector of the atomic system does indeed come about as a result of the interaction between this system and a macroscopic measuring

apparatus when the entire measuring process, consisting of the interaction between the atomic system and apparatus and the subsequent evolution of the apparatus, resulting in the formation of a macroscopic signal, is treated on the basis of quantum mechanics.

A model of the measuring process has been provided by Daneri, Loinger and Prosperi<sup>3)</sup> (referred to as the "Italian group") who have developed a time-independent ergodic theory<sup>5)</sup> which they use to describe the behaviour of the measuring apparatus. Their analysis shows how the reduction of the state vector of the atomic system takes place as a result of the interaction between the atomic system and a macroscopic measuring apparatus and the subsequent recording of the information by the apparatus. The irreversible nature of this change in the state of the atomic system is entirely due to the macroscopic character of the apparatus and the nature of the recording process.

More recently George, Prigogine and Rosenfeld<sup>4)</sup> (referred to as the "Belgian group") have provided a time-dependent theory of large quantal systems which gives a characterization of the macroscopic level of description of such systems. This theory is also used to describe the measurement process in quantum mechanics.

The aim of this thesis is to compare the approach of the Italian group to the consistency problem, with the approach of the Belgian group, and to investigate whether they are equivalent.

## 2. ERGODIC THEORY OF LARGE QUANTAL SYSTEMS

### 2.1 Macroscopic Observables

The considerations below briefly indicate the type of observables corresponding to macroscopic measurements which may be made on a large body (one composed of many (e.g.  $10^{23}$ ) particles).

Such a measurement has an accuracy much more limited than that imposed by the uncertainty relations of quantum mechanics and determines only an interval of values of a number of microscopic observables, therefore a macroscopic measurement does not determine a state vector for the system but only a manifold of state vectors. Since, according to experience, macroscopic measurements may be carried out simultaneously without reciprocal limitations on the accuracy of the measurements, the result of carrying out simultaneously all the macroscopic measurements possible with the greatest possible accuracy, is to determine a manifold of state vectors which represents the maximum information about the system obtainable by measurements of this type. These manifolds, which are referred to as "cells", effect a subdivision of the Hilbert space of the system into orthogonal subspaces.

In the ergodic theory of the Italian group (ref. <sup>3</sup>) sect. 9) the macroscopic description is outlined as follows:

One macroscopic observable is the "energy" of the system and it is assumed that a measurement of this observable determines an interval

$$(E_a, E_{a+1}) = (E_a, E_a + \Delta E) \quad (2.1.1)$$

of values of the unperturbed hamiltonian  $H^{(0)}$  of the system. The choice of  $H^{(0)}$  depends on the system concerned. For example, in a weakly coupled gas,  $H^{(0)}$  is chosen to be the hamiltonian corresponding to non-interacting particles. The manifold of eigenstates of  $H^{(0)}$  whose eigenvalues lie in the interval  $(E_a, E_{a+1})$  is denoted by  $C_a$  and is referred to as the energy shell corresponding to that particular specification of the macroscopic energy. It is assumed that  $\Delta E$  is large enough for  $C_a$  to coincide practically with the manifold of eigenstates, of the complete hamiltonian  $H$ , with eigenvalues in the interval  $(E_a, E_{a+1})$ . This ensures that each energy shell is practically invariant.

There may be further macroscopic constants of the motion. (The existence of at least one other macroscopic constant will be an essential requirement for the system to serve its purpose as a measuring apparatus.) These macroscopic constants will be denoted collectively by  $J$  and will be treated as a single observable. The spectrum of  $J$  can also be divided up into intervals

$$(J_k, J_{k+1}) = (J_k, J_k + \Delta J) \quad (2.1.2)$$

This generates a subdivision of each energy shell  $C_a$  into subspaces  $C_{ak}$  (referred to as "channels") corresponding to the intervals  $(J_k, J_{k+1})$  of eigenvalues of  $J$ .

Concerning the remaining (non-invariant) macroscopic

observables, the most accurate measurement of these observables determines a subspace of  $C_{ak}$  denoted by  $C_{akv}$ , where  $v$  is a collective index denoting an interval of values for each of these observables. The subspace  $C_{akv}$  is referred to as a "cell". A statement as to which cell the state vector of the system is in would be a complete macroscopic specification of the state of the system. The macroscopic description is therefore only concerned with the occupation probability of the cells  $C_{akv}$ .

Each macroscopic observable is therefore of the form

$$A = \sum_{akv} \alpha_{akv} P_{[akv]} \quad , \quad (2.1.3)$$

where  $P_{[akv]}$  denotes the projection operator onto the cell  $C_{akv}$  and  $\alpha_{akv}$  is the eigenvalue of  $A$  associated with that cell. Let  $\{\Omega_{akvi}\}$  be a basis such that the set of vectors  $\{\Omega_{akvi}\}_i$  ( $a, k, v$  fixed) spans the cell  $C_{akv}$ .

The "coarse-graining projection operator" (more precisely a superoperator)  $\mathcal{C}$  defined by

$$\mathcal{C}A = \sum_{akv} \alpha_{akv} P_{[akv]} A = \sum_{akv} \{ \text{tr} P_{[akv]} \}^{-1} \text{tr} (P_{[akv]} A) P_{[akv]} \quad , \quad (2.1.4)$$

where  $A$  is any operator, will be used in the comparison between the ergodic and superspace theories.

The problem of the choice of the macroscopic observables (equivalently the cell subdivision) has not been solved in general, but the following are a few criteria for the choice of these observables for familiar systems:

The hamiltonian for the system may be written as

$$H = H^{(0)} + H^{(1)}, \quad (2.1.5)$$

where the unperturbed part  $H^{(0)}$  is assumed to give a complete separation of variables and would therefore, taken alone, produce no approach to thermodynamic equilibrium. The perturbation  $H^{(1)}$  mixes the many degrees of freedom left uncoupled by  $H^{(0)}$  and is entirely responsible for the irreversible behaviour of the system. The following are a few examples:

1. Non-conducting crystal:  $H^{(0)}$  contains the harmonic part of the forces while  $H^{(1)}$  describes the anharmonic part.
2. Electron-phonon system in metals:  $H^{(0)}$  describes the free harmonic vibrations of the lattice and the conducting electrons in the periodic field of the ions at their equilibrium positions, while  $H^{(1)}$  describes the intermolecular interactions.
3. Dilute gas:  $H^{(0)}$  describes a gas of non-interacting molecules while  $H^{(1)}$  is the potential of the intermolecular forces.

When  $H^{(1)}$  is considered to be a sufficiently small perturbation, the basis of eigenstates of  $H^{(0)}$  seems to be of special significance. If the statistical assumption is made that the system is homogeneous, the macroscopic observables are usually chosen to be diagonal in this representation.

In other words, the basis  $\{\Omega_{akvi}\}$  could be chosen to coincide with the set of eigenstates of  $H^{(0)}$ . For such systems the off-diagonal matrix elements of the density operator refer only to correlations between the excitations (phonons in example 1., phonons and electrons in 2., molecules in 3.). These vary on a very short (atomic) time scale and can not be regarded as being observable at the macroscopic level.

For the case of a dilute gas, the way in which the cells are constructed may be described briefly as follows:

First consider a single particle in a rectangular box. The different wave-number vectors  $\underline{k}$  form a lattice of points in three-dimensional  $\underline{k}$  space. These points can be grouped into energy shells  $C_a$  corresponding to the interval  $(E_a, E_a + \Delta E)$  of kinetic energy. These energy shells are approximately spherical for sufficiently high energies. Each shell is then divided into smaller volumes, approximately cubic, and such that each "cube" has the thickness of the energy shell it is in. Each "cube" in a particular energy shell corresponds to roughly the same size interval of values of  $k_x$ ,  $k_y$  and  $k_z$ . Although  $\Delta E$  is small on the macroscopic scale each "cube" is large enough to contain very many lattice points. For this system each cube defines a "cell" in the Hilbert space of the system and each lattice point in the cube corresponds to a basis vector for the cell. Thus the eigenstates  $|\underline{k}\rangle$  have been grouped together on the basis of similarity of properties associated with energy and momentum components rather than simply in terms of energy only. This can be generalised to the case of a gas of  $N$  particles by considering the  $3N$ -



dimensional wave-vector space.

For the case of an inhomogeneous system and systems for which long-range correlations are relevant to the macroscopic description, the basis of eigenstates of  $H^{(0)}$  is no longer suitable for the cell subdivision because the macroscopic observables are no longer simultaneously diagonal in this representation. A new basis has to be constructed such that each basis vector corresponds, in the case of a gas for example, to partial information on the positions and momenta of the particles.

Consider, for example, the case of a gas or a liquid:

Let  $L_h$  denote a characteristic length on the hydrodynamical scale.  $L_h$  is characteristic of the macroscopic inhomogeneities and long-range correlations.

Let  $L_m$  denote a characteristic length on the atomic scale.  $L_m$  may be chosen to be the range of the forces between the particles.

Consider  $L'$  such that

$$L_m \ll L' \ll L_h \quad . \quad (2.1.6)$$

Consider the volume  $\Omega$ , of the  $N$ -particle system, subdivided into cubes of volume  $(L')^3$ . Now consider  $K'$  satisfying the equation

$$K' L' = \frac{1}{2} \hbar \quad , \quad (2.1.7)$$

and let the three-dimensional wave-vector space be subdivided into cubes of volume  $(K')^3$ . According to von Neumann (ref. <sup>2</sup>) ch. 5, sect. 4) a complete set  $|\chi\rangle$  of single-particle states can be found such that each  $|\chi\rangle$  represents a state in which the particle is in a particular cube in co-ordinate space and a particular cube in wave-vector space. (Here  $\chi$  denotes a suitable set of indices referring to the cubes in question.) This set is not orthogonal, but a complete orthogonal set  $\{|\chi'\rangle\}$  can be obtained from it by application of the E. Schmidt orthogonalization process, such that for each state  $|\chi'\rangle$ , the uncertainties in the variables  $\underline{r}$  and  $\underline{p}$  are still of the order of  $L'$  and  $K'$  respectively. For the one-dimensional case, von Neumann claims (ref. <sup>2</sup>) p. 407) that these uncertainties are greater than  $L'$  and  $K'$  respectively, by a factor of the order of one or two powers of ten.

From the basis  $\{|\chi'\rangle\}$  for a single particle, a basis  $\{|\chi_N\rangle\}$  of N-particle states can be constructed where each  $|\chi_N\rangle$  is a properly symmetrized product of single-particle states  $|\chi'\rangle$ . Each  $|\chi_N\rangle$  would then be characterized by the occupation numbers of the cubes in co-ordinate and momentum space.

A description of the system in terms of probabilities for the states  $|\chi_N\rangle$  would include inhomogeneities and correlations on the hydrodynamical scale  $L_h$ . If  $L'$  is chosen to be closer to the hydrodynamical scale than to the atomic scale the dispersion  $K'$  of the momentum in state  $|\chi\rangle$  would then be very small (since  $K' = \hbar/2L'$ ), even on the microscopic

scale, so that as far as the macroscopic level is concerned, the description in terms of probabilities for the states  $|\chi_N\rangle$  includes the macroscopic description in terms of the probabilities for the eigenstates of  $H^{(0)}$ . The description in terms of probabilities for the states  $|\chi_N\rangle$  is still a fine-grained one. The cell subdivision is performed in a way analogous to that for a homogeneous system except now on the basis of similarity of properties in both configuration and momentum space.

For the theory of the measuring apparatus it is, however, not necessary to discuss the problem of constructing the cell subdivision for inhomogeneous systems.

## 2.2 Ergodic Behaviour and Approach to Equilibrium

In the theory that follows, time averaging over an infinite period is used. The motivation for this (ref. <sup>6</sup>) p. 11) is as follows:

Since macroscopic measurements require a time interval  $T$ , very large compared with time intervals involved in atomic processes, and since the macroscopic observables were chosen to evolve on such a long time scale, the time average of any quantity, over a time interval of duration  $T$ , is all that is relevant when relating the macroscopic description to the microscopic behaviour of the system. Now it is known from experience that a macroscopic system, once all connections with the surroundings have been cut, will tend to an equilibrium state in which it will persist indefinitely except

for small fluctuations. The time average will be the same over any time interval  $T$  except during an initial period of relaxation. Since ergodic theory is not concerned with the relaxation process, the equilibrium state of the system may be defined by extending the time average over an infinite time interval. This time average, extending over all the macroscopic states the system actually passes through, is independent of the order in which they have been passed; it is therefore equivalent to an ensemble average defined by a distribution indicating the relative frequencies of occurrence of the various states. This distribution characterizes the equilibrium state of the system. It is the purpose of ergodic theory to provide this distribution and to explain in what sense the system tends to the equilibrium state described by this distribution.

The macroscopic body is treated as a spatially limited system composed of a large but finite number of particles. The energy spectrum (total or unperturbed) of the system is therefore discrete even though the density of the levels is very high owing to the large number of degrees of freedom and to the large spatial extension of the system. The general solution of the Schrödinger equation is therefore a Fourier series in time and is consequently an almost periodic function of the time. In addition the microscopic laws of dynamics are time-reversal invariant, which implies that for any motion, the time-reversed motion is also possible.

It is one of the basic problems of statistical mechanics to overcome the apparent conflict between the irreversible

behaviour at the macroscopic level and the reversible behaviour at the atomic level. Mathematical considerations alone do not provide a satisfactory solution to the problem and a certain approach to the interpretation of the theory seems to be essential. The problem of the recurrence, mentioned above, can be dispelled by the fact that the period for the recurrence is of the order of  $1/\delta E$ , where  $\delta E$  gives a measure of the spacing between the energy levels of the system. For typical systems  $\delta E$  is so small that the period may be regarded as being of infinite length.

Ergodic theory is not concerned with the temporal behaviour of the macroscopic phenomena, but rather with the justification of the approach to equilibrium and the statistical properties of the state of equilibrium (e.g. the microcanonical ensemble). The purpose of the theory is to provide the conditions under which the time average, over an infinite time interval, of the occupation probability of the various phase cells, may be replaced by a statistical average defined by a stationary distribution over the phase cells.

This distribution must be independent of all the details of the initial state of the system, other than the information concerning the macroscopic constants of the motion.

It is also essential that the statistical fluctuation of any macroscopic observable be very small at equilibrium - say of the order of  $N^{-1}$  where  $N$  is the number of degrees of freedom. (This is required by any theory of statistical mechanics. It is also a necessary requirement for understanding how macroscopic irreversibility can exist in

contrast with the reversible phenomena on the atomic scale, since the statistical irreversibility expressed by ergodic theory is asymptotic (ref. <sup>6</sup>) p. 5).)

### The Ergodic Theory of the Italian Group

Suppose the system is observed, at time  $t = 0$ , to be in the macrostate defined by the cell  $C_{ak\mu}$ , i.e. the state vector  $\Psi(0)$  is in the cell  $C_{ak\mu}$ .  $\Psi(0)$  will therefore be of the form

$$\Psi(0) = \sum_{\mu i} \alpha_{\mu i} \Omega_{k\mu i} \quad , \quad (2.2.1)$$

where the suffix  $a$  has been dropped for convenience of notation.

Let  $U_{kv}(t)$  denote the probability of finding the system in the macrostate  $C_{kv}$  at time  $t$ .

$$U_{kv}(t) = \sum_{i=1}^{S_{kv}} |(\Omega_{kv i}, e^{-\frac{i}{\hbar} H t} \Psi(0))|^2 \quad , \quad (2.2.2)$$

where  $S_{kv}$  denotes the dimension of the cell  $C_{kv}$ . Conditions are required under which, in a subsequent observation, the system will be in some cell  $C_{ke_k}$  with a probability very close to unity and independent of the initial microstate  $\Psi(0)$ . The cell  $C_{ke_k}$  will then be the equilibrium macrostate of the channel  $C_k$ . If  $M$  denotes time averaging, i.e.

$$M = \lim_{T \rightarrow \infty} \int_0^T dt \quad , \quad (2.2.3)$$

the above requirement is equivalent to

$$M U_{kv}(t) \approx \delta_{ve_k} \quad (2.2.4)$$

Clearly, since

$$0 \leq u_{kv}(t) \leq 1 \quad \forall t, \quad (2.2.5)$$

the condition that

$$M U_{kv}(t) \approx \begin{cases} 1 & v = e_k \\ 0 & v \neq e_k \end{cases} \quad (2.2.6)$$

is equivalent to

$$u_{kv}(t) \approx \begin{cases} 1 & v = e_k \\ 0 & v \neq e_k \end{cases}, \quad (2.2.7)$$

for almost all  $t > 0$ .

Let  $S_k$  denote the dimension of channel  $C_k$  and  $S_{kv}$  the dimension of the cell  $C_{kv}$ . The following ergodicity conditions, introduced by the Italian group<sup>5)</sup> are sufficient for the above requirements:

$$M \left\{ \sum_{i=1}^{S_{kv}} |(\Omega_{kv i}, e^{-\frac{i}{\hbar} H t} \Omega_{k \mu j})|^2 \right\} \approx \frac{S_{kv}}{S_k} \quad (2.2.8)$$

$$M \left\{ \sum_{i=1}^{S_{kv}} (\Omega_{kv i}, e^{-\frac{i}{\hbar} H t} \Omega_{k \mu j})^* (\Omega_{kv i}, e^{-\frac{i}{\hbar} H t} \Omega_{k \mu' j'}) \right\} \approx \frac{S_{kv}}{S_k} \delta_{\mu \mu'} \delta_{j j'} \quad (2.2.9)$$

with the following additional requirements:

$$\frac{S_{kv}}{S_k} \ll 1 \quad (v \neq e_k), \quad \frac{S_{ke_k}}{S_k} \approx 1 \quad (2.2.10)$$

Conditions (8) and (9) express the ergodic behaviour of the state vector  $\Psi(t)$  in each channel  $C_k$  and are assumed to hold for all values of  $k$ .

With  $\Psi(0)$  as defined by eq. (1) and  $U_{kv}(t)$  by eq. (2),

$$\begin{aligned} M U_{kv}(t) &= M \sum_{i=1}^{S_{kv}} |(\Omega_{kvi}, e^{-\frac{i}{\hbar} H t} \Psi(0))|^2 \\ &= M \sum_{i=1}^{S_{kv}} |(\sum_{\mu_j} \alpha_{k\mu_j} (\Omega_{kvi}, e^{-\frac{i}{\hbar} H t} \Omega_{k\mu_j}))|^2 \\ &= M \sum_i \sum_{\mu_j} \sum_{\mu'_j} \alpha_{k\mu_j} \alpha_{k\mu'_j}^* (\Omega_{kvi}, e^{-\frac{i}{\hbar} H t} \Omega_{k\mu_j}) (\Omega_{kvi}, e^{-\frac{i}{\hbar} H t} \Omega_{k\mu'_j})^* \\ &\approx M \sum_i \sum_{\mu_j} |\alpha_{k\mu_j}|^2 |(\Omega_{kvi}, e^{-\frac{i}{\hbar} H t} \Omega_{k\mu_j})|^2 \quad (2.2.11) \\ &\approx \left[ \sum_{\mu_j} |\alpha_{k\mu_j}|^2 \right] \frac{S_{kv}}{S_k} = \frac{S_{kv}}{S_k} = \delta_{ve_k} \quad (2.2.12) \end{aligned}$$

as required. The condition

$$\sum_{\mu_j} |\alpha_{k\mu_j}|^2 = 1, \quad (2.2.13)$$

expressing the normalization of  $\Psi(0)$ , as well as the conditions



(8) and (10), were used to obtain eq. (12), and condition (9) was used to obtain eq. (11). Thus the ergodicity conditions (8) and (9), and condition (10), are sufficient to ensure that

$$U_{k\omega}(t) \approx \delta_{\omega} e_k \quad (2.2.14)$$

for almost all  $t > 0$ .

In density operator notation, if

$$\rho(0) = |\Psi(0)\rangle\langle\Psi(0)| \quad , \quad (2.2.15)$$

then

$$\rho(t) = e^{-\frac{i}{\hbar}Ht} |\Psi(0)\rangle\langle\Psi(0)| e^{\frac{i}{\hbar}Ht} \quad (2.2.16)$$

Since for a macroscopic observable  $A$  as given by eq. (2.1.3) we have that  $A = CA$ , where  $C$  is the coarse-graining projection superoperator defined by eq. (2.1.4),

$$\langle A \rangle = \text{tr}(\rho A) = \text{tr}(\rho CA) = \text{tr}(C\rho CA) \quad , \quad (2.2.17)$$

where the last equality uses the fact that  $C$  is a projector. This shows that the "macroscopic part" of  $\rho$  is given by  $C\rho$ .

Now

$$\text{tr}(P_{[\alpha k' \omega]} \rho(t)) = U_{k' \omega}(t) \quad , \quad (2.2.18)$$

therefore, from eqs. (2.1.4), (1) and (12), and using the fact that  $\psi(t)$  is confined to the channel  $C_k$ , the following results are obtained:

For almost all  $t > 0$ ,

$$\begin{aligned} C \rho(t) &= \sum_{k'v} \frac{1}{S_{k'v}} U_{k'v}(t) P_{[k'v]} \\ &= \sum_v \frac{1}{S_{kv}} U_{kv}(t) P_{[kv]} \end{aligned} \quad (2.2.19)$$

$$= \sum_v \frac{1}{S_{kv}} \frac{S_{kv}}{S_k} P_{[kv]} = \frac{1}{S_k} \sum_v P_{[kv]}, \quad (2.2.20)$$

or from eq. (19)

$$C \rho(t) \approx \sum_v \frac{1}{S_{kv}} \delta_{ve_k} P_{[kv]} = \frac{1}{S_{ke_k}} P_{[ke_k]}, \quad (2.2.21)$$

for almost all  $t > 0$ . The index  $a$  was dropped for convenience of notation.

Condition (9) expresses the assumption that the correlations in the system at time  $t = 0$  do not contribute to the macroscopic description, in the sense that the time average of  $U_{kv}(t)$ , for any cell  $C_{kv}$ , is independent of the initial correlations. The idea is that this is true not only for the time average over an infinite time but over any time interval of duration  $T$  (where  $T$  is of the order of the time needed for a macroscopic measurement on the system), provided the interval taken is outside the period of relaxation of the apparatus.

Conditions (8) and (9) together express the assumption that the state of the system in the course of its evolution over a very long time interval is such that the total time it spends in each cell is proportional to the dimension of that cell. This justifies the use of the microcanonical ensemble, restricted to the channel  $C_k$ , (polymicrocanonical ensemble), as the equilibrium distribution, as expressed by eq. (20). Condition (10) is asymptotic in the sense that it is assumed to be true only for a very large system, the inequalities becoming equalities in the limit of an infinite system. This condition has not been proved in general, but in the case of a weakly coupled many-body system the cell corresponding to the Fermi-Dirac or Einstein-Bose distribution has this property (ref. <sup>3</sup>) p. 310). For a classical system composed of  $N$  components and with a separable hamiltonian,

$$H(P) = \sum_{i=1}^N H_i(P_i) \quad , \quad (2.2.22)$$

it has been proved (ref. <sup>7</sup>) that the microcanonical dispersion of any sum-function,

$$F(P) = \sum_{i=1}^N F_i(P_i) \quad , \quad (2.2.23)$$

tends to zero as  $N$  tends to infinity, under certain additional conditions on  $H(P)$  and  $f(P)$ .

Ergodicity conditions (8) and (9) are rather restrictive in the sense that they apply to all initial conditions. Less restrictive ones would apply to the overwhelming majority

of initial conditions, for it is possible in principle that the system can be prepared in an initial state such that it will subsequently show non-thermodynamical behaviour (e.g. by inverting the velocities of the particles of a system that has been behaving thermodynamically). These ergodicity conditions do not anticipate such an ordering of the system at the atomic level.

Under such circumstances, the macroscopic description in terms of ergodic theory would not be relevant. It is emphasized that the purpose of statistical mechanics is to show that the state of a system, when its constituents are free to evolve and interact with one another according to the laws of mechanics, tends statistically towards macrostates of greater and greater probability. On the basis of a macroscopic measurement at one instant, the macroscopic laws express what we may expect the result of a future measurement to be. The irreversibility in the macroscopic description therefore does not conflict with the reversibility of the microscopic description. They are complementary descriptions which apply to different conditions of observation (ref. <sup>6</sup>) p. 5). Under the conditions of macroscopic observation the observer has extremely limited control over the variables describing the motion of the particles, and on the basis of the knowledge he has about a very few controllable quantities, he is only able to make statistical predictions about these quantities.

### 3. RESOLUTION OF THE MEASUREMENT PROBLEM BY THE APPROACH OF THE ITALIAN GROUP

#### 3.1 Example of a Typical Measuring Process

Consider the measurement of the energy of a charged particle by means of a proportional counter:

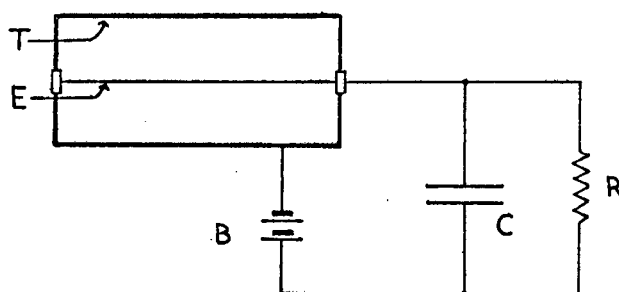


FIG. 1. Schematic representation of a proportional counter

T - tube (cathode)

B - battery (of voltage  $U_0$ )

E - central electrode (anode)

C - condenser

R - resistor (which serves to reset the counter after each count)

(The following description is taken from ref. <sup>3</sup>) sects. 8 and 10.)

The macroscopic constant of the motion,  $U$ , is the average potential difference between the two electrodes when the gas in the tube is in thermal equilibrium and the electrodes are in electrostatic and thermal equilibrium. Here a particular value  $U_k$  refers to an interval  $(J_k, J_k + \Delta J)$  where  $J$  denotes the fine-grained potential difference - a quantity which

fluctuates and which is thus only measured macroscopically with an error greater than  $\Delta J$ .

The energy of the apparatus is assumed to have been macroscopically determined to be in the interval  $(E, E + \Delta E)$ , and the system is initially at equilibrium and charged to a given potential  $U_0$ . The charged particle goes through the counter producing a number of ions, determined within limits by the velocity of the particle. This interaction takes place within a short time interval  $\tau$ . The apparatus is now in a non-equilibrium state corresponding to a new value  $U_k$  of the constant  $U$ . At this instant the macroscopic state of the apparatus is characterized by the average potential difference between the electrodes, which is still  $U_0$ , the number of ions and by the spatial and energetic distributions of the neutral ions and molecules. This transition needs an exchange of energy which is negligible on the macroscopic scale, hence the state vector of the apparatus does not move into a different energy shell.

The electrons produced by the passage of the charged particle migrate towards the central electrode (anode) producing secondary ions. The total number of ions and electrons produced is determined, within limits, by the number of ions and electrons initially produced by the charged particle. The apparatus now evolves spontaneously towards equilibrium, and when all the electrons produced have reached the central anode, the potential difference between the anode and cathode has dropped from  $U_0$  to  $U_k$  where  $U_k$  is given by

$$U_k = U_0 - \frac{e\lambda}{c} N, \quad (3.1.1)$$

where  $N$  is the number of ions and  $e$ ,  $\lambda$  and  $C$  are respectively the elementary charge, the ion multiplication coefficient and the electrostatic capacity of the counter and condenser together. The new potential difference  $U_k$  is thus approximately a function of the velocity of the charged particle as it passed through the tube.

In practice, the drop in potential is amplified and registered by electronic instruments connected to the electrodes, but this further amplification has a relaxation time quite different from the discharge time of the tube and hence need not be included in this description of the apparatus. The transition of the state of the apparatus from channel  $U_0$  to channel  $U_k$  is already a macroscopic change, and the further stages in the measurement process, involving the electronic apparatus, is not essential to this theory.

Denote by  $C_0$  the invariant channel corresponding to the initial value  $U_0$  of the constant  $U$ , and by  $C_k$  the channel corresponding to the value  $U_k$ .  $C_{ke_k}$  denotes the equilibrium manifold corresponding to the situation in which there is thermal equilibrium within the gas and within the electrodes, there are no ions in the gas and the voltage is  $U_k$ . A non-equilibrium manifold  $C_{kv}$  corresponds to a situation in which the voltage is  $U_k$  and no ion is present in the gas, but the gas and the electrodes are not in thermal equilibrium, or to situations in which there is a fixed number,  $N$ , of electrons in the tube and the voltage has the value  $U$  given by

$$U = U_k + \frac{e\lambda}{C} N \quad (3.1.2)$$

### 3.2 General Theory of the Measuring Process

The theory given in this section is based on the work of the Italian group given in ref. <sup>3</sup>).

Let  $A$  be the observable of interest of the atomic system under consideration. Assume, for convenience of notation, that the spectrum of  $A$  is discrete and non-degenerate. In line with the example given in section 3.1, the apparatus is assumed to be, at time  $t = 0$ , in a state  $\Phi_0$  in the equilibrium cell  $C_{oe_0}$  of the channel  $C_0$ . If the particle is in the state  $\phi_k$  (where  $\phi_k$  is an eigenstate of  $A$ ), the interaction between the apparatus and object brings the apparatus into a state  $\Phi_k \in C_k$ . The apparatus is assumed to be ergodic in each channel  $C_k$ , hence its free evolution takes it into the equilibrium cell  $C_{ke_k}$ . (In the example of the proportional counter this corresponds to the migration of the electrons to the anode and the establishment of thermal equilibrium in the gas, electrostatic and thermal equilibrium in the electrodes.)

Let the initial state of the atomic system be given by

$$\phi(0) = \sum_k c_k \phi_k \quad . \quad (3.2.1)$$

Therefore the initial state of the combined system, apparatus + atomic system, is given by

$$\Psi(0) = \sum_k c_k \phi_k \Phi_0 \quad . \quad (3.2.2)$$

The interaction between the two systems lasts for a short



time  $\tau$ . It is assumed that the time scale on which the eigenstates  $\phi_k$  vary and the time scale on which the apparatus evolves is very much longer than  $\tau$  so that  $\phi_k$  and  $\Phi_k$  are almost stationary over the time interval during which the interaction occurs. If  $\phi_k$  does change during the time interval  $\tau$ , a corresponding error occurs in the measurement of A.

The hamiltonian for the combined system may be written as

$$H_{I+II} = H_I + H_{II} + H_{INT} \quad , \quad (3.2.3)$$

where  $H_I$  and  $H_{II}$  describe the free evolution of the atomic system (I) and apparatus (II) respectively, and  $H_{INT}$ , which is effective only during the time interval  $(0, \tau)$ , describes the interaction between systems I and II (e.g. the production of ions in the tube of the proportional counter as the charged particle passes through the tube). The considerations of the previous paragraph are expressed by

$$H_{INT} \gg H_I + H_{II} \quad . \quad (3.2.4)$$

Hence

$$\begin{aligned} \Psi(\tau) &= e^{-\frac{i}{\hbar}(H_I + H_{II} + H_{INT})\tau} \sum_K c_K \phi_K \Phi_0 \\ &\approx e^{-\frac{i}{\hbar}H_{INT}\tau} \sum_K c_K \phi_K \Phi_0 \\ &= \sum_K c_K (e^{-\frac{i}{\hbar}H_{INT}\tau} \phi_K \Phi_0) \quad , \end{aligned} \quad (3.2.5)$$

where the last equality holds by virtue of the linearity of the evolution operator. From the above considerations concerning the interaction between systems I and II, eq. (5) can be written as

$$\Psi(\tau) = \sum_k c_k \phi_k \bar{\Phi}_k \quad . \quad (3.2.6)$$

In the case of a continuous spectrum for the observable A, the spectrum can be considered to be divided into intervals of the form

$$I_i = (a_i, a_i + \delta a) = (a_i, a_{i+1}) \quad . \quad (3.2.7)$$

This subdivision depends on the apparatus and the way it interacts with the atomic system. This generates a subdivision of the Hilbert space of the atomic system into orthogonal subspaces spanned by the sets  $S_i$  given by

$$S_i = \{ \phi_a : a \in I_i \} \quad . \quad (3.2.8)$$

In this case the initial state of the atomic system is given by

$$\phi(o) = \sum_i \phi_i \quad , \quad \phi_i = \sum_{a \in I_i} (\phi_a, \phi(o)) \phi_a \quad , \quad (3.2.9)$$

and each  $\phi_i$  plays the role of one of the  $\phi_k$  in the case of a discrete spectrum.

Returning to eq. (6), the state of the combined system,

at a later time  $t > \tau$ , is given by

$$\begin{aligned}\Psi(t) &= e^{-\frac{i}{\hbar}(H_I + H_{II})t} \sum_K c_K \phi_K \bar{\Phi}_K \\ &= \sum_K c_K e^{-\frac{i}{\hbar}H_I t} \phi_K e^{-\frac{i}{\hbar}H_{II} t} \bar{\Phi}_K.\end{aligned}\quad (3.2.10)$$

Now the description of the apparatus at the macroscopic level is only concerned with the probability of finding the state vector of the apparatus in some cell  $C_{rv}$  (where  $r$  denotes a particular value of the constant of the motion and  $v$  the remaining macroscopic observables). The probability of finding, at any time  $t > 0$ , the atomic system in the state  $\chi$  and the apparatus in the cell  $C_{rv}$  is given by

$$\begin{aligned}U(\chi, c_{rv}; t) &= \sum_{i=1}^{S_{rv}} |(\chi \Omega_{rvi}, \Psi(t))|^2 \\ &= \sum_{i=1}^{S_{rv}} |(\chi \Omega_{rvi}, \sum_K c_K e^{-\frac{i}{\hbar}H_I t} \phi_K e^{-\frac{i}{\hbar}H_{II} t} \bar{\Phi}_K)|^2\end{aligned}\quad (3.2.11)$$

$$= \sum_{i=1}^{S_{rv}} \left| \sum_K c_K (\chi, e^{-\frac{i}{\hbar}H_I t} \phi_K) (\Omega_{rvi}, e^{-\frac{i}{\hbar}H_{II} t} \bar{\Phi}_r) \delta_{rK} \right|^2 \quad (3.2.12)$$

$$= |c_r|^2 |(\chi, e^{-\frac{i}{\hbar}H_I t} \phi_r)|^2 \left\{ \sum_{i=1}^{S_{rv}} |(\Omega_{rvi}, e^{-\frac{i}{\hbar}H_{II} t} \bar{\Phi}_r)|^2 \right\}, \quad (3.2.13)$$

where eq. (10) was used to obtain eq. (11) while eq. (12) results from the invariance of the channels  $C_K$ .

From the considerations of section 2.2, in particular the result expressed by eq. (2.2.14), the term in brackets  $\{\}$  in eq. (13), for values of  $t$  larger than the relaxation time of the apparatus, may be replaced by  $\delta_{ve_r}$ . Thus eq. (13) becomes, for large  $t$ ,

$$U(x, C_r; t) = |c_r|^2 |(x, e^{-\frac{i}{\hbar} H t} \phi_r)|^2 \delta_{ve_r}, \quad (3.2.14)$$

which is independent of the initial phase relations between the different states  $\phi_k$ , and independent of any quantity referring to the apparatus, other than the factor  $\delta_{ve_r}$  which indicates that the apparatus is in the equilibrium state corresponding to the channel  $C_r$ .

This result may be expressed in density operator notation as follows:

Let  $\rho^I$ ,  $\rho^{II}$  and  $\rho^{I+II}$  denote respectively the density operators for the atomic system, apparatus and combined system.

Using the bra-ket notation

$$\begin{aligned} \rho^{I+II}(0) &= |\Psi(0)\rangle \langle \Psi(0)| \\ &= \sum_{\kappa \kappa'} c_{\kappa} c_{\kappa'}^* |\phi_{\kappa}\rangle \langle \phi_{\kappa'}| \cdot |\Phi_0\rangle \langle \Phi_0|. \end{aligned} \quad (3.2.15)$$

At time  $t = \tau$ , using eq. (6),

$$\rho^{I+II}(\tau) = \sum_{\kappa \kappa'} c_{\kappa} c_{\kappa'}^* |\phi_{\kappa}\rangle \langle \phi_{\kappa'}| \cdot |\Phi_{\kappa}\rangle \langle \Phi_{\kappa'}|. \quad (3.2.16)$$

From eq. (10) for  $t > \tau$

$$\begin{aligned} \rho^{I+II}(t) &= \sum_{\kappa\kappa'} c_{\kappa} c_{\kappa'}^* e^{-\frac{i}{\hbar} H_I t} |\phi_{\kappa}\rangle \langle \phi_{\kappa'}| e^{\frac{i}{\hbar} H_I t} e^{-\frac{i}{\hbar} H_{II} t} |\bar{\phi}_{\kappa}\rangle \langle \bar{\phi}_{\kappa'}| e^{\frac{i}{\hbar} H_{II} t} \\ &= \sum_{\kappa\kappa'} c_{\kappa} c_{\kappa'}^* \rho_{\kappa\kappa'}^I(t) \rho_{\kappa\kappa'}^{II}(t) \end{aligned} \quad (3.2.17)$$

Since the macroscopic description of the apparatus is only concerned with the occupation probability  $U_{\kappa\nu}(t)$  for the different cells  $C_{\kappa\nu}$ , and since the matrix elements of the operator  $\rho_{\kappa\kappa'}^{II}(t)$  for  $\kappa \neq \kappa'$  are off-diagonal for all  $t$  in the basis  $|\Omega_{\kappa\nu i}\rangle$  (since  $|\phi_{\kappa}\rangle$  and  $|\bar{\phi}_{\kappa'}\rangle$  are in different invariant manifolds),  $\rho_{\kappa\kappa'}^{II}(t)$  is irrelevant to the macroscopic description of the apparatus. Equivalently it is easy to show that

$$C \rho_{\kappa\kappa'}^{II}(t) = 0 \quad \forall t, \quad \kappa \neq \kappa', \quad (3.2.18)$$

where  $C$  is the coarse-graining superoperator defined by eq. (2.1.4).

Hence from eq. (17) we have that  $\rho^{I+II}(t)$  is equivalent to the expression

$$\tilde{\rho}^{I+II}(t) = \sum_{\kappa} |c_{\kappa}|^2 \rho_{\kappa\kappa}^I(t) \cdot C \rho_{\kappa\kappa}^{II}(t) \quad (3.2.19)$$

By virtue of eq. (2.2.21) regarding  $C \rho_{\kappa\kappa}^{II}(t)$ , eq. (19) may be written as

$$\tilde{\rho}^{I+II}(t) = \sum_{\kappa} |c_{\kappa}|^2 \rho_{\kappa\kappa}^I \frac{1}{S_{\kappa e_{\kappa}}} P_{[\kappa e_{\kappa}]} \quad (3.2.20)$$

This is equivalent to the result expressed by eq. (14) but is much more convenient for the comparison with the Belgian approach. One obtains from eq. (20) an expression for the density operator  $\rho^I(t)$  referring to the atomic system alone by taking the trace of the components referring to the apparatus. This amounts to averaging over the apparatus states, and yields the expression

$$\begin{aligned}\rho^I(t) &= \sum_{\kappa} |c_{\kappa}|^2 \rho^I(t) \frac{1}{S_{\kappa e_{\kappa}}} \text{tr } P_{[\kappa e_{\kappa}]} \\ &= \sum_{\kappa} |c_{\kappa}|^2 \rho_{\kappa\kappa}^I(t) \quad ,\end{aligned}\tag{3.2.2}$$

or, by rewriting  $\rho_{\kappa\kappa}^I(t)$  in full,

$$\rho^I(t) = \sum_{\kappa} |c_{\kappa}|^2 e^{-\frac{i}{\hbar} H_I t} |\phi_{\kappa}\rangle \langle \phi_{\kappa}| e^{\frac{i}{\hbar} H_I t} \quad ,\tag{3.2.2}$$

which is independent of any quantity referring to the apparatus and which is consistent with the reduction rule of quantum mechanics as given in Chapter 1.

It is not always the case that the cells  $C_{\kappa e_{\kappa}}$  correspond to permanent equilibrium states, but they may refer to transient macrostates of sufficient duration for the result of the measurement to be recorded (by some other macroscopic process), or observed directly (For example, in the case of a spark chamber (ref. <sup>8</sup>)), the spark may be observed directly). The requirement that the manifolds  $C_{\kappa}$  are constants of the

motion, is replaced by the condition that the transition probability between states in different manifolds  $C_k, C_{k'}$ , is sufficiently weak for the apparatus to indicate the result of the measurement sufficiently accurately, in the sense that the signal produced by the apparatus is strongly correlated with the state of the atomic system that triggered the apparatus.

The ergodic approach described above does not deal with this more general situation, but it can be shown that the decay of the transient macrostate, being a much slower process than the atomic interactions that gave rise to it, may be easily separated from the latter processes. For a time interval shorter than the decay time of a transient state, of the kind considered here, the channels  $C_k$  are effectively invariant, and the ergodic approach given above is valid over such a time interval, provided the second ergodicity condition, expressed by eq. (2.2.9), is modified to become

$$|M\{\sum_{i=1}^{S_{k\nu}} (\Omega_{k\nu i}, e^{-\frac{i}{\hbar} H t} \Omega_{k'\mu j})^* (\Omega_{k\nu i}, e^{-\frac{i}{\hbar} H t} \Omega_{k''\mu' j'})\}|$$

$$\approx \frac{S_{k\nu}}{S_k} \delta_{jj'} \delta_{kk'} \delta_{k'k''} \delta_{\mu\mu'} \quad (3.2.2)$$

Following the interpretation, given in section 2.2, of the operation of time averaging,  $M$ , condition (23) expresses the assumption that the correlations, at time  $t = 0$ , expressed by a phase relation between the state vectors  $\Omega_{k'\mu j}$  and  $\Omega_{k''\mu' j'}$  (in different channels  $C_{k'}, C_{k''}$ ), does not contribute to the

occupation probability of the cell  $C_k$  after a sufficiently long time  $t$ . Up to now this was a trivial result of the strict invariance of the channels  $C_k$ , but it now has to be stated as an assumption, due to the fact that the channels are not strictly invariant in this case.

This discussion is relevant to the theory of measurement since it concerns the step from eq. (11) to eq. (13). It is in this step that the initial phase relations between the state vectors  $\phi_k$ , pertaining to the atomic system, are eliminated, as can be seen by the fact that eq. (11) involves the coefficients  $C_k$  while eq. (13) involves only  $|C_k|^2$ . This step employed only the invariance of the channels and not the ergodicity conditions (2.2.8) and (2.2.9). It might appear that the reduction of the state vector,  $\phi$ , could be achieved without the ergodicity conditions, but without these conditions, the macroscopic description, in terms of the cell subdivision, is meaningless. Secondly, the apparatus has to be shown to tend to equilibrium, thereby producing a signal at the macroscopic level to indicate the result of the measurement - an essential requirement for the macroscopic system to serve its purpose as a measuring apparatus.

When the manifolds  $C_k$  are not strictly invariant, the step from eq. (11) to eq. (13) must be made using ergodicity condition (23). This emphasises the idea that it is the ergodic nature of the evolution of the apparatus, after it has been triggered by the interaction with the atomic system, that is responsible for the reduction of the state vector of the atomic system.



## 4. SUPERSPACE THEORY OF LARGE QUANTAL SYSTEMS

### 4.1 Basic Modes

In the study of quantal systems composed of many particles, it is usually convenient to consider the hamiltonian  $H$  separated into an unperturbed part  $H^{(0)}$  and a perturbation  $H^{(1)}$ , where the eigenstates of  $H^{(0)}$ , forming a complete orthogonal basis of representation in Hilbert space, represent certain basic modes convenient for a description of the system. Typical examples were given in section 2.1.

This decomposition gives rise to a complete dynamical description of the system in terms of certain generalized co-ordinates and their conjugate momenta, in such a way that  $H^{(0)}$  is a function of the momenta only.  $H^{(1)}$  may be a function of both co-ordinates and momenta. The precise mode of description of the system is relevant to the formulation of the assumptions that are made on the time behaviour of the system, but otherwise the physical results of the theory are independent of the basis of representation.

The theory is concerned with systems having such a large number of degrees of freedom that this number may be taken as infinite, and consequently the volume of the system as infinite. As a result, the energy spectrum of  $H^{(0)}$  (and that of  $H$  as well) will be a continuum, with possibly a discrete set of eigenstates embedded in it (ref. <sup>4</sup>) p. 9). Both possibilities can be incorporated in the notation

$$H^{(0)} = \hbar \int \nu^{(0)}(m) |m\rangle dm \langle m| \quad , \quad (4.1.1)$$

where  $m$  is an infinite set of quantum numbers which labels a basis state of the system. As an example, for a gas of identical particles, writing the vectors  $\underline{k}$  as scalars for convenience of notation,

$$|m\rangle = |\{n_k\}\rangle, \quad (4.1.2)$$

where  $n_k$  is the occupation number of the momentum state  $\hbar k$ , and where the vectors  $k$  are continuously variable. In the case of a solid,  $n_k$  may refer to the number of phonons in state  $\hbar k$ .

#### 4.2 Liouville Equation

In quantum mechanics, the state of a system may be described by the state vector

$$|\Psi(t)\rangle = \sum_m c_m |m\rangle \quad (4.2.1)$$

in Hilbert space, or equivalently, by the density operator

$$\rho(t) = |\Psi(t)\rangle\langle\Psi(t)| = \sum_{mm'} c_m c_{m'}^* |m\rangle\langle m'|, \quad (4.2.2)$$

corresponding to the pure state  $|\Psi(t)\rangle$ . The time evolution of this state is governed by the Schrödinger equation for  $|\Psi(t)\rangle$ , or equivalently, for the density operator, by the Liouville equation

$$i\dot{\rho}(t) = \frac{1}{\hbar} [H, \rho(t)] \quad (4.2.3)$$

More generally, the density operator can be used to describe statistical ensembles of systems and in the study of large quantal systems is much more convenient than the description in terms of the state vector. The density operator describes density distributions in states and correlations between pairs of states. This makes possible the approach of the Belgian group in which the time evolution is given in terms of a "dynamics of correlations", (ref. <sup>9</sup>) p. 6), in which the correlations play the role of dynamical variables.

Referring to the basis  $\{|m\rangle\}$  introduced in section 4.1, eq. (3) can be written as

$$i \frac{\partial}{\partial t} \langle m | \rho | m' \rangle = \frac{1}{\hbar} \sum_{m''} \{ \langle m | H | m'' \rangle \langle m'' | \rho | m' \rangle - \langle m | \rho | m'' \rangle \langle m'' | H | m' \rangle \} \quad (4.2.4)$$

(where, in the limit of an infinite system, the summation is to be replaced by an integration).

Eq. (4) describes the evolution of the system in terms of transitions between the basis states  $|m\rangle$ .

The considerations of the rest of this section are taken from ref. <sup>10</sup>) pp. 542-547.

Introduce new variables  $v$  and  $N$  (to be understood as representing infinite sets of indices of the same form as  $m$ ) given by

$$v = m - m' \quad , \quad N = \frac{1}{2}(m + m') \quad . \quad (4.2.5)$$

A matrix element  $\langle m | A | m' \rangle$  becomes  $\langle N + \frac{1}{2}v | A | N - \frac{1}{2}v \rangle$  and is written as  $A_v(N)$ . Eq. (4) then becomes

$$i \frac{\partial}{\partial t} \rho_{\nu}(N) = \frac{1}{\hbar} \sum_{\nu'} \{ H_{\nu-\nu'}(N + \frac{\nu'}{2}) \rho_{\nu'}(N + \frac{\nu-\nu'}{2}) - H_{\nu-\nu'}(N - \frac{\nu'}{2}) \rho_{\nu'}(N - \frac{\nu-\nu'}{2}) \} \quad (4.2.6)$$

Introducing the operators  $\eta^{\pm \nu}$  such that for any function  $f(N)$ ,

$$\eta^{\pm \nu} f(N) = f(N \pm \frac{\nu}{2}) \quad , \quad (4.2.7)$$

eq. (6) becomes

$$i \frac{\partial}{\partial t} \rho_{\nu}(N) = \sum_{\nu'} \langle \nu | \mathcal{H}(N) | \nu' \rangle \rho_{\nu'}(N) \quad , \quad (4.2.8)$$

where  $\langle \nu | \mathcal{H}(N) | \nu' \rangle$  is an operator in  $N$ -space defined by

$$\langle \nu | \mathcal{H}(N) | \nu' \rangle = \frac{1}{\hbar} [ \eta^{\nu'} H_{\nu-\nu'}(N) \eta^{-\nu} - \eta^{-\nu'} H_{\nu-\nu'}(N) \eta^{\nu} ] \quad (4.2.9)$$

Eq. (8) is formally diagonal in  $N$  and describes the evolution of the system in terms of transitions between matrix elements  $\rho_{\nu}(N)$  with different coefficients  $\nu$  and with the same coefficient  $N$ . Nonzero matrix elements  $\rho_{\nu}(N)$ , for  $\nu \neq \{0\}$ , describe spatial correlations and/or inhomogeneities in the system. In the case of a gas of fermions, for example, consider the expression for the binary correlation function in the formalism of second quantization,

$$n_2(r_1, r_2) = \text{tr} [\Psi^+(r_1) \Psi^+(r_2) \Psi(r_2) \Psi(r_1) \rho] \quad (4.2.10)$$

where, for convenience of notation,  $\underline{r}_1$  and  $\underline{r}_2$  are written as scalars, and where  $\Psi^+$  and  $\Psi$  denote the field creation and annihilation operators respectively.

Expand  $\Psi(r)$  in plane waves as follows:

$$\Psi(r) = \frac{1}{\Omega^{\frac{1}{2}}} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (4.2.11)$$

where  $a_{\mathbf{k}}$  is the annihilation operator for the momentum state  $\hbar\mathbf{k}$ . Using eq. (11), eq. (10) becomes

$$n_2(r_1, r_2) = \frac{1}{\Omega^2} \sum_{\mathbf{k}, \mathbf{l}, \mathbf{p}, \mathbf{r}} e^{i(\mathbf{r}-\mathbf{k}) \cdot \mathbf{r}_1} e^{i(\mathbf{p}-\mathbf{l}) \cdot \mathbf{r}_2} \text{tr}[a_{\mathbf{k}}^+ a_{\mathbf{l}}^+ a_{\mathbf{p}} a_{\mathbf{r}} \rho] \quad (4.2.12)$$

Now

$$\begin{aligned} \text{tr}[a_{\mathbf{k}}^+ a_{\mathbf{l}}^+ a_{\mathbf{p}} a_{\mathbf{r}} \rho] &= \sum_{nn'} \langle n | a_{\mathbf{k}}^+ a_{\mathbf{l}}^+ a_{\mathbf{p}} a_{\mathbf{r}} | n' \rangle \langle n' | \rho | n \rangle \\ &= \sum_{\mathbf{v}} [a_{\mathbf{k}}^+ a_{\mathbf{l}}^+ a_{\mathbf{p}} a_{\mathbf{r}}]_{\mathbf{v}}(N) \rho_{-\mathbf{v}}(N) \end{aligned} \quad (4.2.13)$$

For  $\mathbf{k} \neq \mathbf{l} \neq \mathbf{p} \neq \mathbf{r}$ , eq. (13) becomes

$$\text{tr}[a_{\mathbf{k}}^+ a_{\mathbf{l}}^+ a_{\mathbf{p}} a_{\mathbf{r}} \rho] = \sum_{\mathbf{N}} [a_{\mathbf{k}}^+ a_{\mathbf{l}}^+ a_{\mathbf{p}} a_{\mathbf{r}}]_{\mathbf{l}_k \mathbf{l}_l - \mathbf{l}_p - \mathbf{l}_r}(N) \rho_{-\mathbf{l}_k - \mathbf{l}_l \mathbf{l}_p \mathbf{l}_r}, \quad (4.2.14)$$

i.e. the binary correlation function is contributed to only by the matrix elements  $\rho_{\mathbf{v}}(N)$  with at most four nonzero coefficients  $v$ . The condition  $\sum_{\mathbf{k}} v_{\mathbf{k}} = 0$  is a consequence of the conservation of the number of particles. In a similar way it can be shown that matrix elements of the form  $\rho_{-\mathbf{l}_k \mathbf{l}_k}$  describe density fluctuations.

In general, it can be shown that matrix elements  $\rho_{\mathbf{v}}(N)$  for which there are four or more nonzero coefficients  $v$

satisfying  $\sum_k k v_k = 0$ , describe homogeneous correlations between two or more particles, while those for which  $\sum_k k v_k \neq 0$  are inhomogeneous terms. Since this theory is to be applied to the description of a measuring apparatus, the considerations for inhomogeneous systems will only be dealt with briefly, since they are not of central interest to the measurement problem in quantum mechanics.

The component  $\rho_0(N)$  gives the probability of the momentum configuration  $N = \{n_k\}$ .

From the above considerations, it can be seen that eq. (8), equivalent to the Liouville equation (3), describes the time evolution of the system in terms of transitions between "states" of different correlation (and for inhomogeneous systems, states of different inhomogeneity), corresponding to matrix elements  $\rho_v(N)$  with different numbers of nonzero coefficients  $v$ . The choice of the basis  $\{|m\rangle\}$ , discussed in section 4.1, defines what is meant by the terms "correlation" and "inhomogeneity".

The dynamics of correlations, discussed in the following sections, leads to a clear physical picture of the mechanism of irreversibility in the behaviour of a large quantal system, which would be much more difficult to obtain in the usual Hilbert space formulation of quantum mechanics.

### 4.3 Mathematical Preliminaries

In this section the concepts of superspace, superoperator and supervector are introduced by means of which the Liouville equation (4.2.3) can be written in the form of a linear

equation, and projection superoperators introduced to exploit this linearity. The following definitions are taken from ref. 4) sect. 2.1.

### Definitions

1. Density operator  $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ , corresponding to the pure state  $|\Psi(t)\rangle$  in the Hilbert space of the system.
2. If  $\mathcal{H}$  denotes the Hilbert space of the system, the corresponding superspace is defined as  $\mathcal{H} \times \mathcal{H}^+$  where  $\mathcal{H}^+$  denotes the dual space of  $\mathcal{H}$ . The density operator  $\rho(t)$  is a vector in  $\mathcal{H} \times \mathcal{H}^+$  as is any operator on  $\mathcal{H}$ . Vectors in superspace will be called supervectors in order to distinguish them from vectors in Hilbert space.
3. For any supervectors  $A$  and  $B$  in superspace, the scalar product is defined as  $\text{tr}(A^+B)$ , where  $A^+$  denotes the Hilbert space operator adjoint to the operator  $A$ . The expectation value of the operator  $A$ , in the state represented by the density operator  $\rho$ , is given by

$$\langle A \rangle = \text{tr}(\rho A) = \text{tr}(\rho^+ A) \quad , \quad (4.3.1)$$

since  $\rho$  is self-adjoint, hence  $\langle A \rangle$  is given by the scalar product of the supervectors  $\rho$  and  $A$ .

4. It is possible to introduce linear superoperators which act on supervectors.

5. For any linear superoperator  $O$ , its adjoint  $O^\dagger$  is defined by the relation

$$\text{tr}[A^\dagger(OB)] = \text{tr}[(O^\dagger A)^\dagger B] \quad . \quad (4.3.2)$$

6. The transposition of a (linear) superoperator  $O$ , denoted by  $AO$ , is defined by the relation

$$\text{tr}[(A^\dagger O)B] = \text{tr}[A^\dagger(OB)] \quad . \quad (4.3.3)$$

From eqs. (2) and (3),

$$(O^\dagger A)^\dagger = A^\dagger O \quad , \quad (4.3.4)$$

or by replacing  $O^\dagger$  by  $O$ ,

$$(OA)^\dagger = A^\dagger O^\dagger \quad , \quad (4.3.5)$$

and since, for any two superoperators  $O$  and  $Q$ ,

$$(OQ)^\dagger = Q^\dagger O^\dagger \quad , \quad (4.3.6)$$

the adjoint of any expression involving products of operators and superoperators is simply obtained by taking the adjoint of each operator and superoperator, and inverting the order of factors in each product.

7. A superoperator  $O$  is said to be factorizable when there



exists a pair of supervectors  $M$  and  $N$  such that for any supervector  $A$ ,

$$OA = MAN \quad . \quad (4.3.7)$$

$O$  is denoted by  $M \times N$  and  $O^\dagger$  by  $M^+ \times N^+$ . The transpose of  $O$  is given by the relation

$$A(M \times N) = (N \times M)A \quad . \quad (4.3.8)$$

If  $O = M \times N$  and  $Q = R \times S$ , then  $OQ = MR \times SN$ , i.e.  $OQ$  is factorizable.

A unitary transformation in  $\mathcal{H}$ , given by the unitary operator  $U$ , is equivalent to a linear transformation in  $\mathcal{H} \times \mathcal{H}^+$  given by the superoperator  $\mathcal{U}$ , where  $\mathcal{U} = U \times U^+$ . Now

$$\begin{aligned} \mathcal{U}^\dagger \mathcal{U} &= (U \times U^+)^\dagger (U \times U^+) = (U^+ \times U)(U \times U^+) \\ &= U^+ U \times U^+ U = 1 \times 1 = 1 \end{aligned} \quad (4.3.9)$$

$$\begin{aligned} &= (U \times U^+)(U^+ \times U) = (U \times U^+)(U \times U^+)^\dagger \\ &= \mathcal{U} \mathcal{U}^\dagger \quad , \end{aligned} \quad (4.3.10)$$

where eq. (9) is obtained from the unitarity of  $U$ . In addition,  $\mathcal{U}^\dagger \mathcal{U} = 1$  since  $UU^+ \times UU^+ = 1 \times 1 = 1$ , using again the unitarity of  $U$ , hence  $\mathcal{U}$  is a unitary superoperator. Using this fact,

$$\text{tr}[(\mathcal{U}A)^\dagger(\mathcal{U}B)] = \text{tr}[(\mathcal{U}^\dagger \mathcal{U} A)^\dagger B] = \text{tr}[A^\dagger B] \quad , \quad (4.3.11)$$

i.e. the scalar product of supervectors is conserved under a unitary transformation in superspace.

8. Define the Liouville superoperator

$$L = \frac{i}{\hbar} [H \times 1 - 1 \times H] \quad , \quad (4.3.12)$$

where  $H$  denotes the hamiltonian of the system. The Liouville equation (4.2.3) becomes

$$i \dot{\rho}(t) = L \rho(t) \quad . \quad (4.3.13)$$

The solution of eq. (13) may be formally written as

$$\rho(t) = e^{-iLt} \rho(0) \quad . \quad (4.3.14)$$

Now

$$T(t) \equiv e^{-iLt} \quad (4.3.15)$$

may be written as

$$T(t) = e^{-\frac{i}{\hbar} H t} \times e^{\frac{i}{\hbar} H t} \quad , \quad (4.3.16)$$

which shows that  $T(t)$  is factorizable. Moreover, since  $L$  is self-adjoint,  $T(t)$  is unitary.

9. A superoperator  $O$  satisfying the condition  $(OA)^+ = OA$ , for any self-adjoint supervector  $A$ , is said to be adjoint-symmetrical.

### Projection Operators and Superoperators

The strict mathematical definition of a projection superoperator  $P$  on  $\mathbb{H} \times \mathbb{H}$  would require  $P$  to satisfy the conditions

1.  $P^2 = P$  (idempotency)
2.  $P = P^+$  (self-adjointness)

Conditions 1. and 2. ensure that, for any density supervector  $\rho$  and observable  $A$ ,

$$(P\rho)^+ = P\rho, \quad (4.3.17)$$

and that

$$\langle A \rangle_{P\rho} = \text{tr}[(P\rho)^+ A] \in \mathbb{R}, \quad (4.3.18)$$

where  $\mathbb{R}$  denotes the set of real numbers.

Now condition 1. and the results (17) and (18) are the only properties of  $P$  required for the purposes of this physical theory. For this reason, condition 1. may be replaced by the weaker condition of adjoint-symmetry introduced in definition 9 above. Note that the usual (factorizable) projection superoperators are adjoint-symmetrical.

A projection superoperator (ref. 4) p. 9) is now defined

as a linear superoperator having the properties of idempotency and adjoint-symmetry. The properties (17) and (18) are still satisfied.

Now

$$\langle A \rangle_{P\rho} = \text{tr}[(P\rho)A] = \text{tr}[\rho(P^\dagger A)] \quad , \quad (4.3.19)$$

but the last expression in eq. (19) is not equal to  $\text{tr}[\rho(PA)]$  unless  $P$  is self-adjoint. However, this form of  $\langle A \rangle_{P\rho}$  is not necessary for the purposes of this physical theory. The above definition of a generalized projection superoperator will be adequate, and will make it possible to derive a projection superoperator, of this type, which defines a macroscopic level of description of the physical system which could not have been done in the Hilbert space representation using only the usual self-adjoint projectors.

#### 4.4 Correlation and Vacuum of Correlations Subspaces

For a given basis  $\{|m\rangle\}$  in Hilbert space, the set of all possible operators of the form  $|m\rangle\langle m'|$  constitutes a complete orthogonal basis of representation in superspace.

Define  $P_m = |m\rangle\langle m|$ . In the limit of a continuous spectrum, this is to be interpreted as

$$P_m = \int_{\epsilon(m)} dm' |m'\rangle\langle m'| \quad , \quad (4.4.1)$$

where  $\epsilon(m)$  denotes an infinitesimal neighbourhood of  $m$ .

Superspace will now be decomposed into two orthogonal

and complementary subspaces, suitable for the development of the physical theory, by the introduction of the projection superoperators  $P_0$  and  $P_C$  (ref. <sup>4</sup>) p. 12). For homogeneous systems for which bulk flow properties are of no concern, these projectors are defined as

$$P_0 = \sum_m P_m \times P_m, \quad (4.4.2)$$

$$P_C = \sum_{m \neq m'} P_m \times P_{m'}, \quad (4.4.3)$$

where the basis  $\{|m\rangle\}$  is that discussed in section 4.1. In the limit of a continuous spectrum, definition (2) is to be interpreted as

$$P_0 = \int \int_{(m', m'') \in \Omega_m} dm' dm'' P_{m'} \times P_{m''}, \quad (4.4.4)$$

where  $\Omega_m$  denotes an infinitesimal neighbourhood of the point  $(m, m)$ . The projector  $P_C$  is to be interpreted along similar lines.

As an example of this decomposition, consider the case of a dilute homogeneous gas. The component  $\rho_0 = P_0 \rho$  of the density supervector  $\rho$  describes only the density distribution over the states  $|m\rangle$ , while  $\rho_C = P_C \rho$  describes only the spatial correlations between the particles. The subspaces defined by  $P_C$  and  $P_0$  are called the correlation subspace and vacuum of correlations subspace respectively.

More generally, for inhomogeneous systems, and systems for which long range-correlations are involved, such as may

occur in dense gases or liquids, the projector  $P_C$  need only include the effects of the short-range correlations (ref. 4) p. 12), and  $P_O$  then includes the inhomogeneities and long-range correlations. The discussion of homogeneous systems is sufficient for the description of the measuring process in this approach to the measurement problem in quantum mechanics, but for the sake of completeness, the decomposition of superspace, in terms of  $P_O$  and  $P_C$ , will be discussed briefly for the more general case of an inhomogeneous system. The projectors  $P_O$  and  $P_C$  will be defined below in a way which makes it possible later to show the equivalence of the macroscopic levels of description of the superspace and ergodic theories.

Referring to the example of an inhomogeneous gas, and to the basis  $\{|\chi_N\rangle\}$  introduced in section 2.1, define  $P_O$  and  $P_C$  as

$$P_O = \sum_{\chi_N} |\chi_N\rangle \langle \chi_N| \quad , \quad (4.4.5)$$

$$P_C = \sum_{\chi_N \neq \chi'_N} |\chi_N\rangle \langle \chi'_N| \quad . \quad (4.4.6)$$

As discussed in section 2.1,  $P_O\rho$  satisfies the above requirement of including macroscopic inhomogeneities and long-range correlations, while  $P_C\rho$  includes the short-range correlations. More precisely, it is important to note that  $P_C\rho$  describes only the short-range correlation effects, since in practice only the two length scales  $L_m$  and  $L_h$  occur, and

inhomogeneities and correlations on some intermediate length scale do not arise.

The superoperators  $P_O$  and  $P_C$ , defined by eqs. (2) and (3), satisfy the requirements, for projectors, of idempotency and adjoint-symmetry, as well as the conditions of complementarity and orthogonality.

Idempotency:

$$\begin{aligned}
 P_O^2 &= \left( \sum_m P_m \times P_m \right) \left( \sum_{m'} P_{m'} \times P_{m'} \right) = \sum_{mm'} (P_m \times P_m) (P_{m'} \times P_{m'}) \\
 &= \sum_{mm'} P_m P_{m'} \times P_{m'} P_m = \sum_{mm'} (P_m \times P_m) \delta_{mm'} = P_O \quad . \quad (4.4.7)
 \end{aligned}$$

where the last line above uses the orthogonality and idempotency of the projectors  $P_m, P_{m'}$ . In the limit of a continuous spectrum, the Kronecka delta  $\delta_{mm'}$  becomes the Dirac delta function  $\delta(m-m')$ .

$$\begin{aligned}
 P_C^2 &= \left( \sum_{m \neq m'} P_m \times P_{m'} \right) \left( \sum_{k \neq k'} P_k \times P_{k'} \right) \\
 &= \sum_{\substack{m \neq m' \\ k \neq k'}} P_m P_k \times P_{k'} P_{m'} = \sum_{\substack{m \neq m' \\ k \neq k'}} (P_m \times P_{m'}) \delta_{mk} \delta_{k'm'} \\
 &= \sum_{m \neq m'} P_m \times P_{m'} = P_C \quad . \quad (4.4.8)
 \end{aligned}$$

Adjoint-symmetry and Complementarity:

obvious from the definitions of  $P_O$  and  $P_C$ .

Orthogonality:

$$\begin{aligned}
 P_O P_C &= \left( \sum_m P_m \times P_m \right) \left( \sum_{k \neq k'} P_k \times P_{k'} \right) \\
 &= \sum_m \sum_{k \neq k'} P_m P_k \times P_{k'} P_m = \sum_m \sum_{k \neq k'} (P_k \times P_{k'}) \delta_{mk} \delta_{k'm} \\
 &= \sum_{k \neq k'} (P_k \times P_{k'}) \delta_{kk'} = 0 \quad . \quad (4.4.9)
 \end{aligned}$$

Similarly  $P_C P_O = 0$ .

4.5 Reduced Properties

The theory of large quantal systems, involving the use of the density operator  $\rho$ , is based on the following considerations:

It is impossible for a macroscopic observer to ascertain the outcome of a single measurement performed on a system whose initial state is macroscopically specified. The only possible prediction is the average result of a large number of such measurements performed on similar macroscopic systems. It is assumed that this averaging process is weighted by the density operator  $\rho$ , which is constructed at the initial time in such a way as to be compatible with the macroscopic information the observer has obtained about the system. The observable value of any macroscopic quantity of interest is



taken to be the average value, weighted with  $\rho$ , of the corresponding microscopic quantity, as follows:

$$\langle A(t) \rangle_{\text{macro}} = \text{tr}[A \rho(t)] = \sum_N A_N(N) \rho_N(N, t) \quad (4.5.1)$$

The classical analogue of eq. (1), in the case of a fluid or a gas, is

$$\langle A(t) \rangle_{\text{macro}} = \int \dots \int (d\mathbf{x})^N (d\mathbf{p})^N A(\{\mathbf{x}_i\}, \{\mathbf{p}_i\}) f_N(\{\mathbf{x}_i\}, \{\mathbf{p}_i\}, t) \quad (4.5.2)$$

where  $f_N$  is the  $N$ -particle distribution function and  $A(\{\mathbf{x}_i\}, \{\mathbf{p}_i\})$  is the dynamical function corresponding to the microscopic observable.

Now the macroscopic description must be such that the outcome of any macroscopic measurement, because of the very large number ( $N$ ) of particles in the system, will be very close (presumably, within an error of order  $N^{-1}$ ) to the average value predicted by the ensemble (given by  $\rho(t)$  or  $f_N(t)$ ). In classical mechanics this is believed to be the case for quantities the dynamical functions of which depend on a small number of co-ordinates and momenta only (ref. <sup>12</sup>) p. 6). These are referred to as reduced quantities. Typical examples are local density, hydrodynamical velocity, local energy density, and binary correlations in velocity or density. Referring to the quantum statistical operator  $A$  corresponding to the reduced classical quantity  $A(\{\mathbf{x}_i\}, \{\mathbf{p}_i\})$  (through the use of Weyl's rule), this means that the only nonzero matrix elements  $A_N(N)$  of the operator  $A$  are those

with only a few nonzero coefficients  $v$ . More precisely, if  $A(\{x_i\}, \{p_i\})$  is a function of  $n$  position co-ordinates  $x_i$ , the only nonzero matrix elements of the operator  $A$  will be those with at most  $2n$  nonzero coefficients  $v$  (ref. <sup>10</sup>) p. 547). In section 4.2 it was shown that the only nonzero matrix elements of the operator corresponding to the binary correlation function  $n_2(r_1, r_2)$  are those with at most four nonzero coefficients  $v$ . Therefore, referring to eq. (1), it is evident that only those matrix elements  $\rho_v(N, t)$ , of the density operator  $\rho(t)$ , with a few nonzero coefficients  $v$  are relevant for calculating the macroscopic quantities at time  $t$ . When the asymptotic limit of an infinite system is taken, the restriction to a "few" degrees of freedom becomes a restriction to a finite number of degrees of freedom.

The above considerations for the matrix elements, in the  $v$ - $N$  notation, of an observable  $A$  corresponding to a reduced quantity, apply not only to a fluid or a gas as considered here, but to any many-particle system. The information contained in  $\rho(t)$  is therefore redundant, and the specification of the macroscopic state at time  $t$  merely amounts to stating some properties of the matrix elements of this type. For this specification to be an adequate macroscopic description of the system, it must be possible to predict, at least approximately, the results of future measurements. For this purpose, some closed description for the time evolution of the relevant matrix elements is therefore necessary. The work of the Belgian group in this direction (e.g. refs. <sup>9, 10</sup>), which provides such a contracted

description, is outlined in sections 4.6 and 4.7.

#### 4.6 Outline of the Approach of the Belgian Group in the v-N

##### Notation

The Liouville equation in the v-N notation, introduced in section 4.2, was given by eq. (4.2.8) as

$$i \frac{\partial}{\partial t} \rho_{\nu}(N, t) = \sum_{\nu'} \langle \nu | \mathcal{H}(N) | \nu' \rangle \rho_{\nu'}(N, t) \quad (4.6.1)$$

The formal solution of eq. (1) is given by

$$\rho_{\nu}(N, t) = \sum_{\nu'} \langle \nu | e^{-i\mathcal{H}(N)t} | \nu' \rangle \rho_{\nu'}(N, 0) \quad (4.6.2)$$

Now

$$e^{-i\mathcal{H}t} = \frac{1}{2\pi i} \oint_C dz \frac{e^{-izt}}{z - \mathcal{H}} \quad (4.6.3)$$

$$= \frac{1}{2\pi i} \oint_C dz e^{-izt} \mathcal{R}(z), \quad (4.6.4)$$

where C is the closed contour in the z plane, enclosing the singularities  $\{z_i\}$  of the resolvent  $\mathcal{R}(z)$ , as shown in fig. 2.

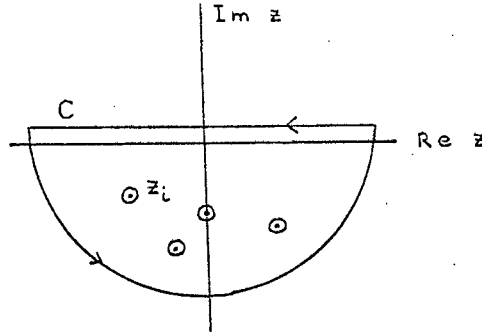


FIG. 2

Using eq. (4), eq. (2) can be written as a pair of coupled equations

$$\rho_0(t) = \frac{1}{2\pi i} \oint_C dz e^{-izt} \{ \langle 0 | R(z) | 0 \rangle \rho_0(0) + \sum_{\nu \neq 0} \langle 0 | R(z) | \nu \rangle \rho_\nu(0) \} \quad (4.6.5)$$

and

$$\rho_\nu(t) = \frac{1}{2\pi i} \oint_C dz e^{-izt} \{ \langle \nu | R(z) | 0 \rangle \rho_0(0) + \sum_{\nu' \neq 0} \langle \nu | R(z) | \nu' \rangle \rho_{\nu'}(0) \} \quad (4.6.6)$$

where, for convenience of notation, the index N has been dropped.

The decomposition  $H = H^{(0)} + H^{(1)}$  gives rise to the decomposition  $\mathcal{H} = \mathcal{H}^{(0)} + \mathcal{H}^{(1)}$ .

Now

$$\begin{aligned} R(z) &= \frac{1}{z - \mathcal{H}} = \frac{1}{z - \mathcal{H}^{(0)} - \mathcal{H}^{(1)}} \\ &= \sum_{n=0}^{\infty} \frac{1}{z - \mathcal{H}^{(0)}} \left[ \mathcal{H}^{(1)} \frac{1}{z - \mathcal{H}^{(0)}} \right]^n \end{aligned}$$

$$= \sum_{n=0}^{\infty} R^{(0)}(z) [H^{(1)} R^{(0)}(z)]^n, \quad (4.6.7)$$

where

$$R^{(0)}(z) = \frac{1}{z - H^{(0)}}. \quad (4.6.8)$$

Using eq. (7), it can be seen that any "matrix element"  $\langle v | R(z) | v' \rangle$  describes a superposition of processes each starting from a correlated state  $v'$  and ending with the state  $v$ , but involving different numbers  $n$  of interactions which give rise to a change of correlation.

For example, consider the term  $n = 2$  in the expansion of  $\langle v | R(z) | v' \rangle$  using eq. (7).

$$\begin{aligned} \langle v | R(z) | v' \rangle_{n=2} &= \langle v | R^{(0)}(z) [H^{(1)} R^{(0)}(z)]^2 | v' \rangle \\ &= \langle v | R^{(0)}(z) H^{(1)} R^{(0)}(z) H^{(1)} R^{(0)}(z) | v' \rangle \\ &= \sum_{v''} \langle v | R^{(0)}(z) | v'' \rangle \langle v'' | H^{(1)} | v''' \rangle \langle v''' | R^{(0)}(z) | v'''' \rangle \langle v'''' | H^{(1)} | v' \rangle \langle v' | R^{(0)}(z) | v' \rangle. \end{aligned} \quad (4.6.9)$$

Expressions of this form appear in the integrand in eqs. (5) and (6).

Using the convolution theorem for Laplace transforms twice, the contribution of such a term to the integral in eqs. (5) and (6) may be written in the following way:

$$\frac{1}{2\pi i} \oint_C dz e^{-izt} \langle \nu | R(z) | \nu' \rangle_{n=2} = \sum_{\nu''} \int_0^t d\tau_2 \int_0^{\tau_2} d\tau_1 \langle \nu | e^{-iH^{(0)}(t-\tau_2)} | \nu'' \rangle \times$$

$$\langle \nu'' | H^{(1)} | \nu'' \rangle \langle \nu'' | e^{-iH^{(0)}(\tau_2-\tau_1)} | \nu'' \rangle \langle \nu'' | H^{(1)} | \nu' \rangle \langle \nu' | e^{-iH^{(0)}\tau_1} | \nu' \rangle \quad (4.6.10)$$

Each term in the summation over  $\nu''$  gives the contribution due to the possible transitions  $\nu' \rightarrow \nu$ , via  $\nu''$  as an intermediate state of correlation of duration  $(\tau_2 - \tau_1)$ .

The term  $\nu'' = 0$  gives the contribution due to the transition which has the vacuum of correlations as an intermediate state.

An irreducible transition, denoted by a suffix irr, is one which does not involve the vacuum as an intermediate state.

The following irreducible transitions (ref. <sup>11</sup>) appendix) are central in the theory:

$$\Psi(z) \equiv \langle 0 | H^{(1)} \sum_{n=1}^{\infty} (R^{(0)}(z) H^{(1)})^n | 0 \rangle_{irr} \quad (4.6.11)$$

$$\Phi_{\nu}(z) \equiv \langle 0 | \sum_{n=1}^{\infty} (H^{(1)} R^{(0)}(z))^n | \nu \rangle_{irr} \quad (4.6.12)$$

$$C_{\nu}(z) \equiv \langle \nu | \sum_{n=1}^{\infty} (R^{(0)}(z) H^{(1)})^n | 0 \rangle_{irr} \quad (4.6.13)$$

$$P_{\nu\nu'}(z) \equiv \langle \nu | R^{(0)}(z) \sum_{n=0}^{\infty} (H^{(1)} R^{(0)}(z))^n | \nu' \rangle_{irr} \quad (4.6.14)$$

The operators defined by eqs. (11), (12), (13) and (14)

are referred to as the irreducible collision operator, destruction (of correlations) operator, creation operator and propagation operator respectively.

The vacuum to vacuum transition  $\langle 0 | R(z) | 0 \rangle$  may be performed in an arbitrary number of collisions (ref. <sup>11</sup>) p. 421). This gives

$$\langle 0 | R(z) | 0 \rangle = \sum_{n=0}^{\infty} \frac{1}{z^{n+1}} [\Psi(z)]^n. \quad (4.6.15)$$

Using the four operators defined by eqs. (11), (12), (13) and (14), similar decompositions of the other transitions appearing in eqs. (5) and (6) are possible (ref. <sup>11</sup>) pp. 421, 422). Eqs. (5) and (6) then become

$$\rho_0(t) = \frac{1}{2\pi i} \oint_C dz e^{-izt} \sum_{n=0}^{\infty} \frac{[\Psi(z)]^n}{z^{n+1}} [\rho_0(0) + \sum_{\nu \neq 0} \mathcal{Q}_{\nu}(z) \rho_{\nu}(0)], \quad (4.6.16)$$

$$\rho_{\nu}(t) = \rho'_{\nu}(t) + \rho''_{\nu}(t), \quad (4.6.17)$$

where  $\rho'_{\nu}$  and  $\rho''_{\nu}$  are defined as

$$\rho'_{\nu}(t) = \frac{1}{2\pi i} \oint_C dz e^{-izt} \sum_{\nu' \neq 0} \mathcal{P}_{\nu\nu'}(z) \rho_{\nu'}(0) \quad (4.6.18)$$

$$\rho''_{\nu}(t) = \frac{1}{2\pi i} \oint_C dz e^{-izt} \mathcal{C}_{\nu}(z) \left\{ \sum_{n=0}^{\infty} \frac{[\Psi(z)]^n}{z^{n+1}} [\rho_0(0) + \sum_{\nu' \neq 0} \mathcal{Q}_{\nu'}(z) \rho_{\nu'}(0)] \right\}. \quad (4.6.19)$$

The set of equations (16) - (19) is equivalent to the Liouville equation. In the limit of an infinite system, under the conditions given below, many simplifications occur

in these equations.

It is required that, in this limit, all local properties (e.g. hydrodynamical variables, intensive thermodynamic properties, binary correlations) have finite values independent of the volume of the system. In the case of a gas, for example, this at least requires the average concentration of particles to be finite. In general this condition is ensured provided the following two conditions, which are the main assumptions of the theory of the Belgian group (ref. <sup>10</sup>) p. 542), are satisfied:

I. The density operator  $\rho(o)$ , taken as the initial condition, must be compatible with the requirement that all reduced properties are finite in this limit. This imposes a certain singularity condition (ref. <sup>10</sup>) p. 550) on the matrix elements  $\rho_v(N,o)$ , concerning their dependence on the volume of the system.

II. At the initial time all spatial correlations must be of finite extension. Physically this assumption means that after a finite time initially correlated particles separate off and thus no longer interact with each other; mathematically, it imposes the requirement that  $\rho_v(N,o) = \rho_{\{v_k\}}(\{N_k\},o)$  be a regular function of the arguments  $k$  (In this limit the summation  $\sum_v$  that occurs in eqs. (16), (18) and (19), is to be interpreted as an integration with respect to the variables  $k$ ).

It can be shown that condition I. is persistent in the course of time (ref. <sup>13</sup>) p. 52).



For a finite system the singularities, in the  $z$  plane, of the expressions  $\Psi(z)$ ,  $\sum_v \vartheta_v(z) \rho_v(0)$  and  $\sum_v \rho_{vv}(z) \rho_v(0)$  all lie on the real axis. The time evolution of the system, given by eqs. (16) - (19), is therefore periodic and no convenient approximations can be made on these equations. As the limit of an infinite system is approached, these singularities become more and more dense, and in the limit, form a finite discontinuity along the real axis (ref. <sup>9</sup>) sects. 4 and 5).

Now in the expressions for  $\Psi(z)$ ,  $\vartheta_v(z)$  and  $\rho_{vv}(z)$ , given by eqs. (11), (12) and (14), summations with respect to coefficients  $v''$  are implied. For example, consider the term  $[\Psi(z)]_{n=1}$  in eq. (11), given by

$$\begin{aligned} [\Psi(z)]_{n=1} &= \langle 0 | \mathcal{H}^{(1)} R^{(0)}(z) \mathcal{H}^{(1)} | 0 \rangle_{\text{irr}} \\ &= \sum_{v''} \langle 0 | \mathcal{H}^{(1)} | v'' \rangle \langle v'' | R^{(0)}(z) | v'' \rangle \langle v'' | \mathcal{H}^{(1)} | 0 \rangle_{\text{irr}} \quad , \quad (4.6.20) \end{aligned}$$

since  $R^{(0)}(z)$  is diagonal in  $v$ . In the limit of an infinite system, the summation with respect to  $v''$  becomes an integral with respect to the variables  $k$  (see condition II. above). Moreover, expression (20) takes the form of a Cauchy integral (ref. <sup>10</sup>) p. 564). This is because the various terms in the sum  $\sum_v$  are regular functions of the variables  $k$ . This in turn is due to the fact that the particles of the system are assumed to interact through short-range forces. Systems of particles interacting through long-range forces require a more

detailed analysis and will not be considered here.

Similarly the other terms  $[\Psi(z)]_n$  in expression (11) can be put into the form of Cauchy integrals. Similar considerations apply to  $\mathcal{D}_v(z)$  and  $\mathcal{P}_{vv}(z)$ . Now condition II. ensures that  $\rho_v(N,0)$  is a regular function of the arguments  $k$ , hence the expressions  $\sum_v \mathcal{D}_v(z) \rho_v(0)$  and  $\sum_v \mathcal{P}_{vv}(z) \rho_v(0)$  also become Cauchy integrals.

Referring now to eqs. (16), (18) and (19), the Cauchy integrals  $\Psi(z)$ ,  $\sum_v \mathcal{D}_v(z) \rho_v(0)$  and  $\sum_v \mathcal{P}_{vv}(z) \rho_v(0)$  are to be evaluated for  $\text{Im } z > 0$ . This is because the solution of the Liouville equation for  $t > 0$  is required. (If the solution for  $t < 0$  is required, these integrals must be evaluated for  $\text{Im } z < 0$ . If there is a difference in the solutions, it is indicative of non-invariance under time-reversal and hence, possibly, of thermodynamic behaviour. It is interesting to see how the asymptotic limit of an infinite system must be taken before the distinction between advanced and retarded solutions appears.)

Because they are Cauchy integrals, these terms are regular functions of  $z$  in the half plane  $\text{Im } z > 0$ . It is assumed that they may be continued analytically into the lower half plane. These continuations must have singularities in the lower half plane otherwise they would be constants. Since only short-range interactions are considered, these singularities will be simple poles. (In the case of a many-body system interacting through long-range forces, such as gravitational or coulomb forces, branch points may occur on the real or imaginary axes (ref. <sup>10</sup>) p. 564).)

Concerning the positions of these poles, only an intuitive argument is possible in this general discussion. If it is assumed that the range of the initial correlations given by  $\rho_v(0)$  is of the order of  $L_m$ , where  $L_m$  denotes a characteristic atomic distance (for example the range of the inter-particle forces),  $L_m$  is the only characteristic length appearing in the terms in question. If it is true that most of the particles have velocities in the neighbourhood of some average velocity  $v$ , then from a dimensional argument (ref. <sup>13</sup>), the poles in question must lie at an effective distance  $\tau_c^{-1}$  below the real axis, where  $\tau_c = L_m/v$  denotes a characteristic collision time scale. In the case of an anharmonic solid  $\tau_c$  would be given by  $\tau_c = a/c$  where  $a$  denotes the lattice distance and  $c$  the velocity of sound in the solid (ref. <sup>9</sup> p. 53).

The main conclusion of this discussion is that the poles of  $\Psi(z)$ ,  $\sum_v \Phi_v(z) \rho_v(0)$  and  $\sum_v \rho_{vv}(z) \rho_v(0)$  lie at a distance of the order of  $\tau_c^{-1}$  below the real axis. Therefore  $\rho'_v(t)$ , given by eq. (18), tends asymptotically to zero with a relaxation time of the order of  $\tau_c$ .

If the range of the initial correlations is of the order of  $L$  say, then  $\rho'_v(t)$  should decay with a relaxation time of the order of  $L/v$ , but it is emphasized that these considerations on the time behaviour of  $\rho'_v(N,t)$  are to be understood as applying to a certain class of observables, namely thermodynamic ones which, as far as correlations are concerned, are only concerned with short-range atomic correlations (ref. <sup>9</sup> pp. 193-195). The matrix elements

$A_{\nu}(N)$  of these observables are therefore regular functions of the arguments  $k$  (see condition II. above). This point is referred to in section 4.12, and in chapter 7 in the comparison with ergodic theory.

In order to develop eqs. (16) - (19) further, it is convenient to use the superspace formalism introduced in sections 4.3 and 4.4. These equations may be rederived in an exactly analogous way using the projectors  $P_0$  and  $P_C$ .

#### 4.7 Superspace Approach

The Liouville equation

$$i \frac{\partial \rho}{\partial t} = L \rho \quad (4.7.1)$$

can be written as a set of coupled Liouville equations (ref.

4) p. 13), using the projectors  $P_0$  and  $P_C$  defined by eqs.

(4.4.2) and (4.4.3), as follows:

$$i \dot{\rho}_0 = L_{00} \rho_0 + L_{0c} \rho_c, \quad (4.7.2)$$

$$i \dot{\rho}_c = L_{c0} \rho_0 + L_{cc} \rho_c, \quad (4.7.3)$$

where  $L_{00} = P_0 L P_0$ ,  $L_{0c} = P_0 L P_C$ ,  $L_{c0} = P_C L P_0$  and

$L_{cc} = P_C L P_C$ .

By application of Laplace transform methods to eq. (3), the solution to this equation can be written as

$$\rho_c(t) = e^{-iL_{cc}t} \left\{ \rho_c(0) - i \int_0^t d\tau e^{iL_{cc}\tau} L_{c0} \rho_0(\tau) \right\}. \quad (4.7.4)$$

Define

$$T_c(t) = e^{-iL_{cc}t}, \quad \gamma_c(z) = -iP_c \frac{1}{LP_c - z}, \quad (4.7.5)$$

where  $\gamma_c(z)$  is the Laplace transform of  $T_c(t)$  such that

$$T_c(t) = \frac{1}{2\pi i} \oint_C dz e^{-izt} \gamma_c(z), \quad (4.7.6)$$

where  $C$  is the contour given in fig. 2.

By definition of  $P_0$  and  $P_c$ , the matrix elements of  $\rho_0$  are of the form  $\rho_0(N)$  while those of  $\rho_c$  are of the form  $\rho_v(N)$  ( $v \neq \{0\}$ ). Now  $T_c(t)$  describes the time evolution starting with  $\rho_c(0)$  and ending with  $\rho_c(t)$  and confined to the correlation subspace. The matrix elements of  $T_c(t) \rho_c(0)$  in the  $v$ - $N$  notation are precisely the terms  $\rho'_v(N,t)$  given by eq. (4.6.18). The considerations of section 4.6 concerning the matrix elements  $\rho'_v(N,t)$  apply directly to  $T_c(t) \rho_c(0)$ , and are summarized by the assumption that for any regular supervector  $A_c$ , not invariant,

$$T_c(t) A_c \xrightarrow[t \rightarrow \infty]{} 0, \quad (4.7.7)$$

with the understanding that this expression decays to zero on a short collision time scale. Assumption (7) is referred to as the asymptotic hypothesis (ref. <sup>14</sup>) p. 1334). The discussion in section 4.6 concerning the singularities of the expression  $\Sigma_v, \rho_{vv}(z) \rho_v(0)$ , applies to  $\gamma_c(z) A_c$  as follows:

For any regular supervector  $A_c$ ,  $\gamma_c(z) A_c$ , defined for

$\text{Im } z > 0$ , is regular in that half plane, and in the asymptotic limit, has a finite discontinuity along the real axis. Continued analytically into the lower half plane,  $\Upsilon_c(z) A_c$  has simple poles at a distance below the real axis depending on the range of the interaction potential and the regularity of  $A_c$ .

This results in the following equivalent expression of the asymptotic hypothesis (c.f. ref. <sup>4</sup>) p. 13):

$$\lim_{z \rightarrow +i0} z \Upsilon_c(z) A_c = 0, \quad (4.7.8)$$

which expresses the assumption that  $\Upsilon_c(z)$  is regular in the vicinity of  $+i0$ .

Except for additional points of clarification (referring to the example of a dilute gas or a fluid), the main results of the rest of this section are taken from ref. <sup>4</sup>) sect. 2.4.

Using eq. (7), eq. (4) becomes

$$\rho_c(t) = -i \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \rho_o(t-\tau) \quad (4.7.9)$$

for large  $t$  (i.e. for  $t \gg \tau_c$ ). Denoting by  $\tilde{\rho}_c(t)$  the asymptotic form of  $\rho_c(t)$  in time,

$$\tilde{\rho}_c(t) = -i \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \rho_o(t-\tau) \quad (4.7.10)$$

Provided  $L_{co} \rho_o(t-\tau)$  is regular, assumption (7) may be applied to the integrand in eq. (10). In the example of a homogeneous gas or fluid, the condition of regularity of an

operator refers to the spatial dependence of the operator (see condition II. in section 4.6). Now the spatial dependence of  $L_{co} \rho_o(t-\tau)$  comes in through the spatial dependence of  $L_{co}$  which involves the short-range forces between the particles. Hence  $L_{co} \rho_o(t-\tau)$  is regular to the extent that the expression

$$I(\tau) = e^{-iL_{cc}\tau} L_{co} \rho_o(t-\tau) \quad (4.7.11)$$

decays to zero on the collision time scale  $\tau_c$ , introduced in section 4.6, because of the short-range spatial dependence of  $L_{co}$ . Hence the integrand in eq. (10) is only appreciable for small values of  $\tau$  and this equation can be written as

$$\tilde{\rho}_c(t) = -i \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \tilde{\rho}_o(t-\tau) \quad (4.7.12)$$

Substituting eq. (12) into eq. (2) and using the  $\sim$  notation to denote asymptotic values,

$$i\dot{\tilde{\rho}}_o(t) = L_{oo}\tilde{\rho}_o(t) - iL_{oc} \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \tilde{\rho}_o(t-\tau) \quad (4.7.13)$$

Eq. (13) can be written as

$$i\dot{\tilde{\rho}}_o(t) = \theta \tilde{\rho}_o(t) \quad (4.7.14)$$

where  $\theta$  is given by

$$\{\theta - L_{oo} + iL_{oc} \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} e^{i\theta\tau}\} \tilde{\rho}_o(t) = 0 \quad (4.7.15)$$

The above integral with respect to  $\tau$  may be extended to an integral over the range  $(0, \infty)$  on the grounds that the superoperator  $\theta$ , describing the asymptotic evolution of  $\rho_0(t)$ , is expected, by construction, to involve only long term transients on a time scale  $t_R \gg \tau_c$ . This results in the following equation for  $\theta$ :

$$\theta = L_{00} - iL_{0c} \int_0^\infty d\tau e^{-iL_{cc}\tau} L_{c0} e^{i\theta\tau} \quad , \quad (4.7.16)$$

which may be solved by iteration as follows:

$\theta = 0$  corresponds to the unperturbed motion  
( $H^{(1)} = 0$ ).

$\theta_1 = \theta(0)$  obtained by substituting  $\theta = 0$  in the  
R.H.S. of eq. (16) corresponds to a system  
for which the collisions may be regarded  
as instantaneous.

etc.

The series obtained by such a scheme must converge on physical grounds for systems exhibiting suitably separated time scales (ref. <sup>14</sup>) pp. 1335, 1336), i.e. provided the asymptotic evolution generated by  $\theta$  is on a long time scale  $t_R \gg \tau_c$ . As can be seen by comparing eqs. (13) and (14),  $\theta$  takes into account the finite duration of the elementary collision processes, since eq. (13) shows explicitly the  $\tau$  integration over a time interval of order  $\tau_c$ , while eq. (14) is of Markovian form.

Eq. (16) may be written as



$$\Theta = L_{oo} + L_{oc} C \quad , \quad (4.7.17)$$

where C is defined by

$$iC = \int_0^\infty d\tau T_c(\tau) L_{co} e^{i\Theta\tau} \quad . \quad (4.7.18)$$

Eq. (12) then becomes

$$\tilde{\rho}_c(t) = C \tilde{\rho}_o(t) \quad . \quad (4.7.19)$$

Eqs. (17) and (18) are a pair of coupled equations and may be used for determining  $\Theta$  and C. C is called the "creation superoperator" (of correlations) since it describes the combined effect of processes leading from a vacuum state to a state of the correlation subspace.

Rewriting eq. (18) as

$$iC = \int_0^\infty d\tau e^{-iL_{cc}\tau} L_{co} e^{i\Theta\tau} \quad , \quad (4.7.20)$$

the following is obtained by partial integration:

$$\begin{aligned} iC &= \left[ \frac{1}{-iL_{cc}} e^{-iL_{cc}\tau} L_{co} e^{i\Theta\tau} \right]_0^\infty - \int_0^\infty d\tau \frac{1}{-iL_{cc}} e^{-iL_{cc}\tau} L_{co}(i\Theta) e^{i\Theta\tau} \\ &= \frac{1}{iL_{cc}} L_{co} + \frac{1}{-iL_{cc}} [-i \int_0^\infty d\tau T_c(\tau) L_{co} e^{i\Theta\tau}] \Theta \quad . \end{aligned} \quad (4.7.21)$$

Multiplying from the left by  $-iL_{cc}$ , this gives

$$L_{cc}C = -L_{co} + C\Theta \quad (4.7.22)$$

i.e.

$$C\theta = L_{co} + L_{cc} C \quad . \quad (4.7.23)$$

Consider the asymptotic equations (14) and (19).  
Substitute eq. (17) into eq. (14). This gives

$$i\dot{\tilde{\rho}}_0(t) = L_{oo}\tilde{\rho}_0(t) + L_{oc} C \tilde{\rho}_0(t) \quad . \quad (4.7.24)$$

Therefore, using eq. (19),

$$i\dot{\tilde{\rho}}_0(t) = L_{oo}\tilde{\rho}_0(t) + L_{oc}\tilde{\rho}_c(t) \quad . \quad (4.7.25)$$

Now from eqs. (19), (14) and (23),

$$\begin{aligned} i\dot{\tilde{\rho}}_c(t) &= iC\dot{\tilde{\rho}}_0(t) = C\theta\tilde{\rho}_0(t) \\ &= L_{co}\tilde{\rho}_0(t) + L_{cc} C \tilde{\rho}_0(t) \quad . \end{aligned} \quad (4.7.26)$$

Therefore, using eq. (19),

$$i\dot{\tilde{\rho}}_c(t) = L_{co}\tilde{\rho}_0(t) + L_{cc}\tilde{\rho}_c(t) \quad . \quad (4.7.27)$$

According to eqs. (25) and (27), the solutions,  $\tilde{\rho}_0(t)$  and  $\tilde{\rho}_c(t)$ , of the asymptotic equations (14) and (19) are exact solutions of the Liouville equations (2) and (3). It is for this reason that it will be possible to define  $\tilde{\rho}_0(t)$

and  $\tilde{\rho}_c(t)$  for all  $t \geq 0$  and to give these supervectors a physical interpretation. Moreover, the form of eq. (14) makes possible a comparison with various kinetic equations (e.g. the Boltzmann equation) previously derived empirically.

At this stage it is convenient to explain the approach of the Belgian group in more detail.

The Liouville equations, expressed in the form of eqs. (14) and (19), can be expanded as a set of coupled equations for the matrix elements  $\rho_v(N,t)$ . This is an infinite set of equations in an infinite number of unknowns, and no solution is possible from this approach. However, equations for the matrix elements  $\rho_v(N,t)$ , relevant to reduced quantities, may be obtained by truncation of this set of equations. One obtains equations for reduced properties depending on one particle, two particles, etc., up to any number of particles depending on the degree of accuracy required (ref. <sup>12</sup>) p. 27). Assumption I. in section 4.6 is essential for this truncation process to work and to yield reduced equations which are independent of the volume of the system. For example, the Boltzmann equation, which describes the evolution of the one-particle density operator may be obtained.

Since eqs. (14) and (19) are asymptotic equations, the solutions  $\tilde{\rho}_o(t)$  and  $\tilde{\rho}_c(t)$  are without any physical interpretation until they are related to  $\rho_o(o)$  and  $\rho_c(o)$ . In sections 4.8 and 4.9 further properties of  $\tilde{\rho}_o(t)$  and  $\tilde{\rho}_c(t)$  are established which give them physical meaning.

#### 4.8 Heisenberg Picture and Time-reversal

(The theory of this section is taken from ref. <sup>4</sup>) sect. 2.5).

In the Heisenberg picture, any time dependent operator  $A(t)$  satisfies the Liouville equation

$$i\dot{A}(t) = -L A(t) \quad , \quad (4.8.1)$$

where  $L$  is time independent.

Time-inversion of a supervector  $A(t)$  and the superoperator  $O(t)$  is defined as follows:

$$\bar{A}(t) = A^\dagger(-t) \quad , \quad \bar{O}(t) = O^\dagger(-t) \quad . \quad (4.8.2)$$

Hence

$$\begin{aligned} i\dot{\bar{A}}(t) &= [-L A(-t)]^\dagger = -A^\dagger(-t)L \\ &= L A^\dagger(-t) = L \bar{A}(t) \quad , \end{aligned} \quad (4.8.3)$$

i.e.  $\bar{A}(t)$  satisfies the Liouville equation. As a result, the asymptotic components  $\tilde{\bar{A}}_O(t) = P_O \tilde{\bar{A}}(t)$  and  $\tilde{\bar{A}}_C(t) = P_C \tilde{\bar{A}}(t)$ , where  $\tilde{\bar{A}}(t)$  denotes the asymptotic form of  $\bar{A}(t)$ , satisfy the equations of motion

$$\tilde{\bar{A}}_O(t) = e^{-i\Theta t} \tilde{\bar{A}}_O(0) \quad (4.8.4)$$

and

$$\tilde{\bar{A}}_C(t) = C \tilde{\bar{A}}_O(t) \quad . \quad (4.8.5)$$

The validity of eqs. (4) and (5) requires the observable  $A(0)$  to be regular. This is the case for thermodynamic

quantities (see the second last paragraph of section 4.6). Note that  $\bar{A}(0) = A^+(0) = A(0)$ , since  $A(0)$  is time independent and  $A$  is self-adjoint, hence  $\bar{A}(0)$  is regular provided  $A(0)$  is regular. The asymptotic equations (4) and (5) therefore apply to  $\bar{A}(t)$  whenever the operator  $A$  refers to thermodynamic quantities.

Define  $\eta = \bar{\Theta}$  and  $D = \bar{C}$ . Taking the time-inverse of eqs. (4.7.17), (4.7.23) and (4.7.18) gives

$$\eta = L_{oo} + D L_{co} \quad (4.8.6)$$

$$\eta D = L_{oc} + D L_{cc} \quad (4.8.7)$$

$$iD = \int_0^\infty d\tau e^{i\eta\tau} L_{oc} T_c(\tau) \quad (4.8.8)$$

In obtaining eq. (8) from eq. (4.7.18) the interval of integration had to be changed from  $(0, \infty)$  to  $(0, -\infty)$ . In general, the operation of time-inversion can be carried out more simply by taking the adjoint and changing the sign of  $L$  wherever it appears.

From eqs. (4.7.17), (4.7.18), (6) and (8)

$$\Theta = L_{oo} - i \int_0^\infty d\tau \bar{\Psi}(\tau) e^{i\Theta\tau} \quad (4.8.9)$$

$$\eta = L_{oo} - i \int_0^\infty d\tau e^{i\eta\tau} \bar{\Psi}(\tau) \quad (4.8.10)$$

where

$$\Psi(t) = L_{oc} T_c(t) L_{co} \quad (4.8.11)$$

Now  $\Psi(t)$  describes an evolution from the vacuum (of correlations) to the vacuum with only correlated states as intermediate states. In other words  $\Psi(t)$  represents irreducible collision processes and is therefore called the irreducible collision operator.

The Laplace transform of  $\Psi(t)$  is given by

$$\Psi_z(z) = L_{oc} \Upsilon_c(z) L_{co} \quad , \quad (4.8.12)$$

where  $\Upsilon_c(z)$  is the Laplace transform of  $T_c(t)$ . ( $\Psi_z(z)$  is the superspace counterpart of  $\Psi(z)$  defined by eq. (4.6.11).)

Let  $N_o = 1 + DC$ , then from eqs. (4.7.17), (4.7.23), (6) and (7),

$$N_o \Theta = \eta N_o \quad (4.8.13)$$

From eqs. (4.7.18), (8) and (11),

$$N_o = 1 - \int_0^\infty d\tau \int_0^\infty d\tau' e^{i\eta\tau} \Psi(\tau + \tau') e^{i\Theta\tau'} \quad (4.8.14)$$

In general  $N_o$  will have an inverse and eq. (13) gives

$$\eta = N_o \Theta N_o^{-1} \quad , \quad \Theta = N_o^{-1} \eta N_o \quad (4.8.15)$$

The asymptotic density supervector  $\tilde{\rho}(t)$  may now be related to the exact density supervector  $\rho(t)$  for all  $t \geq 0$  as follows:

The time evolution of  $\tilde{\rho}_0(t)$  is given by eq. (4.7.14) or equivalently by

$$\tilde{\rho}_0(t) = e^{-i\theta t} \tilde{\rho}_0(0) \quad . \quad (4.8.16)$$

Hence, from eq. (13),

$$N_0 \tilde{\rho}_0(t) = N_0 e^{-i\theta t} \tilde{\rho}_0(0) = e^{-i\eta t} N_0 \tilde{\rho}_0(0) \quad . \quad (4.8.17)$$

From eqs. (6) and (7)

$$\eta(P_0 + D) = (P_0 + D)L \quad . \quad (4.8.18)$$

Hence

$$\begin{aligned} i \frac{\partial}{\partial t} [(P_0 + D)\rho(t)] &= (P_0 + D) i \frac{\partial}{\partial t} \rho(t) \\ &= (P_0 + D)L \rho(t) \\ &= \eta(P_0 + D)\rho(t) \quad ,/ \end{aligned} \quad (4.8.19)$$

or equivalently

$$(P_0 + D)\rho(t) = e^{-i\eta t} (P_0 + D)\rho(0) \quad . \quad (4.8.20)$$

Comparing eqs. (17) and (20), it can be seen that if the initial condition for  $\tilde{\rho}_0$  is chosen as

$$\tilde{\rho}_0(o) = N_o^{-1} [\rho_o(o) + D \rho_c(o)] \quad , \quad (4.8.21)$$

then this relation holds for all later times  $t$ , and is the required relationship between  $\tilde{\rho}_0(t)$  and  $\rho(t)$ . This can be shown as follows:

$$\begin{aligned} N_o \tilde{\rho}_0(t) &= e^{-i\eta t} N_o \tilde{\rho}_0(o) \\ &= e^{-i\eta t} N_o N_o^{-1} [\tilde{\rho}_0(o) + D \rho_c(o)] \\ &= e^{-i\eta t} (P_o + D) \rho(o) \\ &= (P_o + D) \rho(t) \\ &= \rho_o(t) + D \rho_c(t) \quad , \end{aligned} \quad (4.8.22)$$

where eqs. (17), (20) and (21) were used. Therefore

$$\tilde{\rho}_0(t) = N_o^{-1} [\rho_o(t) + D \rho_c(t)] \quad \forall t \geq 0 \quad , \quad (4.8.23)$$

as required.

In sect. 4.9 further properties of  $\tilde{\rho}(t)$  and its time evolution are derived (following ref. <sup>4</sup>) sect. 2.7) which make it possible to provide a macroscopic level of description for the system.



#### 4.9 The Projectors $\tilde{\Pi}$ and $\hat{\Pi}$ and Subdynamics

Using eq. (4.7.19)

$$\begin{aligned}
 (P_0 + C)\tilde{\rho}(t) &= (P_0 + C)(\tilde{\rho}_0(t) + \tilde{\rho}_c(t)) \\
 &= (P_0 + C)\tilde{\rho}_0(t) \\
 &= \tilde{\rho}_0(t) + \tilde{\rho}_c(t) \\
 &= \tilde{\rho}(t) \quad , \quad (4.9.1)
 \end{aligned}$$

i.e.  $\tilde{\rho}(t)$  is contained in the subspace defined by the projection superoperator  $P_a = P_0 + C$ . That  $P_a$  is a projector can be seen as follows:

Idempotency:

$$\begin{aligned}
 P_a^2 &= (P_0 + C)^2 = P_0^2 + P_0 C + C P_0 + C^2 \\
 &= P_0 + 0 + C + 0 = P_a \quad . \quad (4.9.2)
 \end{aligned}$$

Adjoint-symmetry:

From eqs. (4.7.17) and (4.7.18) it can be seen that  $C$  is a functional of  $iL$ . Now  $iL$  is adjoint-symmetrical since for any self-adjoint supervector  $A$ ,

$$\begin{aligned}
 (iLA)^+ &= -iA^+L^\dagger \\
 &= -iAL = iLA \quad , \quad (4.9.3)
 \end{aligned}$$

where the last equality follows from the fact that  $L$  changes sign on transposition, hence  $C$  is adjoint-symmetrical as well. Since  $P_0$  is adjoint-symmetrical ( $P_0$  is a projector), so is  $P_0 + C$ .

Similarly  $P_b = P_c - C$  is a projection superoperator.

Now

$$\begin{aligned} P_a P_b &= (P_0 + C)(P_c - C) \\ &= P_0 P_c + C P_c - P_0 C - C^2 = 0 \end{aligned} \quad (4.9.4)$$

Similarly  $P_b P_a = 0$ , hence  $P_b$  defines a subspace of superspace, orthogonal (and complementary) to that defined by  $P_a$ .

Similarly  $\bar{P}_a = P_0 + D$  and  $\bar{P}_b = P_0 - D$  are projection superoperators which define orthogonal and complementary subspaces of superspace. (Recall from sect. 4.8 that the notation  $\bar{\phantom{x}}$  denotes time-reversal.)

Now define

$$N_c = 1 + CD \quad (4.9.5)$$

The following relations are of interest:

$$\bar{P}_a P_a = P_0 N_0 = N_0 P_0 \quad P_b \bar{P}_b = P_c N_c = N_c P_c \quad (4.9.6)$$

$$P_a P_0 = P_0 \quad P_0 \bar{P}_0 = \bar{P}_0 \quad P_c P_b = P_b \quad \bar{P}_b P_c = \bar{P}_b \quad (4.9.7)$$

Note that  $\theta$  and its time-inverse  $\eta$  may be written as

$$\theta = P_0 L P_a \quad , \quad \eta = \bar{P}_a L P_0 \quad . \quad (4.9.8)$$

Eq. (4.8.18) and its time-inverse give

$$\eta \bar{P}_a = \bar{P}_a L \quad , \quad P_a \theta = L P_a \quad (4.9.9)$$

respectively. Define the superoperators  $\zeta$  and  $\lambda$  by

$$\zeta = P_c L \bar{P}_b \quad , \quad \lambda = P_b L P_c \quad . \quad (4.9.10)$$

(Clearly  $\zeta = \bar{\lambda}$ .) They satisfy the relations

$$\bar{P}_b \zeta = L \bar{P}_b \quad , \quad \lambda P_b = P_b L \quad . \quad (4.9.11)$$

From eq. (4.8.13) and its time-inverse,

$$N_0 \theta = \eta N_0 \quad , \quad N_c \zeta = \lambda N_c \quad . \quad (4.9.12)$$

Now from eqs. (4.7.19), (4.8.16) and (4.8.23)

$$\begin{aligned} \tilde{\rho}(t) &= (P_0 + C) \tilde{\rho}_0(t) = P_a \tilde{\rho}_0(t) \\ &= P_a e^{-i\theta(t-t_0)} \tilde{\rho}_0(t_0) \quad 0 \leq t_0 \leq t \\ &= P_a e^{-i\theta(t-t_0)} N_0^{-1} [ \rho_0(t_0) + D \rho_c(t_0) ] \\ &= P_a e^{-i\theta(t-t_0)} N_0^{-1} \bar{P}_a \rho(t_0) \quad , \end{aligned} \quad (4.9.13)$$

i.e.

$$\tilde{\rho}(t) = \tilde{\Sigma}(t - t_0) \rho(t_0) \quad , \quad (4.9.14)$$

where

$$\tilde{\Sigma}(t) \equiv P_a e^{-i\theta t} N_o^{-1} \bar{P}_a \quad \forall t \geq 0 \quad . \quad (4.9.15)$$

From eq. (12)  $\Theta N_o^{-1} = N_o^{-1} \eta$ , therefore

$$\tilde{\Sigma}(t) \equiv P_a N_o^{-1} e^{-i\eta t} \bar{P}_a \quad \forall t \geq 0 \quad . \quad (4.9.16)$$

Now the R.H.S. of eq. (16) is the time-inverse of the R.H.S. of eq. (15), therefore  $\tilde{\Sigma}(t)$  is invariant under time-reversal.

Furthermore, using eqs. (6),

$$\begin{aligned} \tilde{\Sigma}(t_1) \tilde{\Sigma}(t_2) &= P_a e^{-i\theta t_1} N_o^{-1} \bar{P}_a P_a e^{-i\theta t_2} N_o^{-1} \bar{P}_a \\ &= P_a e^{-i\theta t_1} N_o^{-1} N_o P_o e^{-i\theta t_2} N_o^{-1} \bar{P}_a \\ &= P_a e^{-i\theta(t_1+t_2)} N_o^{-1} \bar{P}_a \\ &= \tilde{\Sigma}(t_1 + t_2) \quad \forall t_1, t_2 \geq 0 \quad . \end{aligned} \quad (4.9.17)$$

Taking the limit  $t_0 \rightarrow t$  in eq. (14),

$$\tilde{\rho}(t) = \tilde{\Pi} \rho(t) \quad , \quad (4.9.18)$$

where

$$\tilde{\Pi} \equiv P_a N_a^{-1} \bar{P}_a \quad . \quad (4.9.19)$$

From eq. (17), taking  $t_1 = t_2 = 0$ ,  $\tilde{\Pi}\tilde{\Pi} = \tilde{\Pi}$  (i.e.  $\tilde{\Pi}$  is idempotent) and since each factor in the expression for  $\tilde{\Pi}$  in eq. (19) is a functional of  $iL$ ,  $\tilde{\Pi}$  is a functional of  $iL$  and is therefore adjoint-symmetrical. Hence  $\tilde{\Pi}$  is a projection superoperator. Since  $\tilde{\Sigma}(t)$  is time-reversal invariant, so is  $\tilde{\Pi}$ .

Also from eq. (17),

$$\tilde{\Sigma}(t) \tilde{\Pi} = \tilde{\Pi} \tilde{\Sigma}(t) = \tilde{\Sigma}(t) \quad . \quad (4.9.20)$$

Now from eqs. (14), (18) and (20),

$$\tilde{\rho}(t) = \tilde{\Sigma}(t-t_0) \tilde{\rho}(t_0) \quad . \quad (4.9.21)$$

From eqs. (9) and (19),

$$P_a \Theta N_a^{-1} \bar{P}_a = L P_a N_a^{-1} \bar{P}_a = L \tilde{\Pi} \quad , \quad (4.9.22)$$

but from eqs. (9) and (12),

$$\begin{aligned} P_a \Theta N_a^{-1} \bar{P}_a &= P_a N_a^{-1} \eta \bar{P}_a \\ &= P_a N_a^{-1} \bar{P}_a L = \tilde{\Pi} L \quad . \end{aligned} \quad (4.9.23)$$

From eqs. (22) and (23),

$$L \tilde{\Pi} = \tilde{\Pi} L, \quad (4.9.24)$$

therefore

$$e^{-iLt} \tilde{\Pi} = \tilde{\Pi} e^{-iLt} = \tilde{\Sigma}(t) \quad (4.9.25)$$

According to eq. (18) and the fact that  $\tilde{\Pi}$  is a projector,  $\tilde{\rho}(t)$  is given, for all  $t \geq 0$ , by the projection of  $\rho(t)$  onto the subspace defined by the projector  $\tilde{\Pi}$ . This subspace is called the "asymptotic subspace", sometimes referred to as the  $\tilde{\Pi}$  subspace. From eq. (25) it can be seen that  $\tilde{\rho}(t)$  is an exact solution of the Liouville equation which now appears as the equation of motion not only in the full superspace, but in the asymptotic subspace as well.

Consider the supervector  $\hat{\Pi}$  defined by

$$\hat{\Pi} = \bar{P}_b N_c^{-1} P_b \quad (4.9.26)$$

The proof that  $\hat{\Pi}$  is a projector is similar to the proof for  $\tilde{\Pi}$ .

Now

$$\hat{\Pi} \tilde{\Pi} = \bar{P}_b N_c^{-1} P_b P_a N_o^{-1} \bar{P}_a = 0 \quad (4.9.27)$$

since  $P_b P_a = 0$ . Similarly  $\tilde{\Pi} \hat{\Pi} = 0$ , therefore  $\tilde{\Pi}$  and  $\hat{\Pi}$  are orthogonal projectors. In addition, using eqs. (6),

$$\begin{aligned}
\bar{P}_a (\tilde{\Pi} + \hat{\Pi}) &= \bar{P}_a P_a N_o^{-1} \bar{P}_a + \bar{P}_a \bar{P}_b N_c^{-1} P_b \\
&= P_o N_o N_o^{-1} \bar{P}_a = P_o \bar{P}_a = \bar{P}_a .
\end{aligned}
\tag{4.9.28}$$

Similarly  $\bar{P}_b (\tilde{\Pi} + \hat{\Pi}) = \bar{P}_b$ , therefore

$$(\bar{P}_a + \bar{P}_b)(\tilde{\Pi} + \hat{\Pi}) = \bar{P}_a + \bar{P}_b , \tag{4.9.29}$$

but  $\bar{P}_a$  and  $\bar{P}_b$  are complementary, hence  $\tilde{\Pi} + \hat{\Pi} = 1$ , i.e.  $\tilde{\Pi}$  and  $\hat{\Pi}$  are complementary projectors.

Define

$$\hat{\rho}(t) = \hat{\Pi} \rho(t) , \tag{4.9.30}$$

therefore from eqs. (11), (12) and (26),

$$\begin{aligned}
\hat{\rho}(t) &= \bar{P}_b N_c^{-1} P_b e^{-iLt} \rho(o) \\
&= \bar{P}_b N_c^{-1} e^{-i\lambda t} P_b \rho(o) \\
&= \bar{P}_b e^{-i\zeta t} N_c^{-1} P_b \rho(o) \\
&= \hat{\Sigma}(t) \rho(o) ,
\end{aligned}
\tag{4.9.31}$$

where  $\hat{\Sigma}(t)$  is defined by

$$\hat{\Sigma}(t) = \bar{P}_b N_c^{-1} e^{-i\lambda t} P_b = \bar{P}_b e^{-i\zeta t} N_c^{-1} P_b \quad (4.9.32)$$

Using eqs. (6),

$$\begin{aligned} \hat{\Sigma}(t_1) \hat{\Sigma}(t_2) &= \bar{P}_b N_c^{-1} e^{-i\lambda t_1} P_b \bar{P}_b N_c^{-1} e^{-i\lambda t_2} P_b \\ &= \bar{P}_b N_c^{-1} e^{-i\lambda t_1} P_b N_c N_c^{-1} e^{-i\lambda t_2} P_b \\ &= \bar{P}_b N_c^{-1} e^{-i\lambda(t_1 + t_2)} P_b \\ &= \hat{\Sigma}(t_1 + t_2) \quad \forall t_1, t_2 \geq 0 \end{aligned} \quad (4.9.33)$$

Now

$$\hat{\Sigma}(t) \hat{\Pi} = \hat{\Pi} \hat{\Sigma}(t) = \hat{\Sigma}(t) \quad , \quad (4.9.34)$$

$$\hat{\Sigma}(t) = e^{-iLt} \hat{\Pi} = \hat{\Pi} e^{-iLt} \quad . \quad (4.9.35)$$

The proof of these relations is similar to the proof of the analogous relations for  $\tilde{\Sigma}(t)$  and  $\tilde{\Pi}$ .

The subspace defined by the projection superoperator  $\hat{\Pi}$  is called the "fluctuation subspace". The fluctuation component  $\hat{\rho}(t)$  of  $\rho(t)$ , given at any time  $t \geq 0$  by the projection of  $\rho(t)$  onto the fluctuation subspace (or  $\hat{\Pi}$  subspace),



is an exact solution of the Liouville equation, as can be seen from eq. (35). The Liouville equation is therefore the equation of motion in the fluctuation subspace as well as in the asymptotic subspace and complete superspace.

The complete dynamical evolution of the system, given in terms of the supervector  $\rho(t)$  in superspace, is thus separated into two independent evolutions (subdynamics), given in terms of the projections,  $\tilde{\rho}(t)$  and  $\hat{\rho}(t)$ , of  $\rho(t)$  onto the subspaces  $\tilde{\Pi}$  and  $\hat{\Pi}$  respectively. Both  $\tilde{\rho}(t)$  and  $\hat{\rho}(t)$ , appearing as exact solutions of the Liouville equation, are confined to their corresponding subspaces. The physical interpretation of the asymptotic and fluctuation subdynamics is given in section 4.12.

#### 4.10 Invariants of the System

Let  $\Phi = \Phi_o + \Phi_c$  be an invariant (constant of the motion) of the system. From eq. (4.8.1) this means that  $L\Phi = 0$ , which is equivalent to the following pair of equations:

$$L_{oo} \Phi_o + L_{oc} \Phi_c = 0 \quad (4.10.1)$$

$$L_{co} \Phi_o + L_{cc} \Phi_c = 0 \quad (4.10.2)$$

From eq. (2), operating from the left by  $-iT_c(\tau)$  and integrating over the interval  $(0, t)$  yields (ref. <sup>4</sup>) p. 24)

$$-i \int_0^t d\tau T_c(\tau) L_{co} \Phi_o + [T_c(t) - 1] \Phi_c = 0 \quad (4.10.3)$$

If  $\phi_c$  is a regular supervector, not itself an invariant, the fundamental asymptotic assumption (4.7.7) (or (4.7.8)) ensures that

$$\lim_{t \rightarrow \infty} T_c(t) \bar{\phi}_c = 0 \quad (4.10.4)$$

as well as the existence of the supervector  $C(0)\phi_0$  with

$$C(0) = -i \int_0^\infty d\tau T_c(\tau) L_{c0} \quad , \quad (4.10.5)$$

since by taking the limit  $t \rightarrow \infty$  in eq. (3), one obtains

$$C(0)\bar{\phi}_0 = \bar{\phi}_c \quad . \quad (4.10.6)$$

Substituting eq. (6) into eq. (1) yields

$$[L_{00} + L_{0c} C(0)] \bar{\phi}_0 = 0 \quad . \quad (4.10.7)$$

This implies (ref. <sup>4</sup>) p. 24) that

$$\Theta \bar{\phi} = 0 \quad . \quad (4.10.8)$$

The proof of eq. (8) is as follows:

Recall eqs. (4.7.18) and (4.7.17) given as

$$C = -i \int_0^\infty d\tau T_c(\tau) L_{c0} e^{i\Theta\tau} \quad (4.10.9)$$

and

$$\theta = L_{oo} + L_{oc} C \quad (4.10.10)$$

respectively, and consider the following solutions for  $C$  and  $\theta$  by iteration:

$$C(o) = -i \int_0^\infty d\tau T_c(\tau) L_{co} \quad \theta_1 = L_{oo} + L_{oc} C(o) \quad (4.10.11)$$

$$C(1) = -i \int_0^\infty d\tau T_c(\tau) L_{co} e^{i\theta_1 \tau} \quad \theta_2 = L_{oo} + L_{oc} C(1) \quad (4.10.12)$$

etc.

From eq. (7)  $\theta_1 \Phi_o = 0$ , i.e.  $\theta_1 \Phi = 0$ , hence from eq. (12)

$$\begin{aligned} C(1) \Phi &= -i \int_0^\infty d\tau T_c(\tau) L_{co} e^{i\theta_1 \tau} \Phi \\ &= -i \int_0^\infty d\tau T_c(\tau) L_{co} \Phi = C(o) \Phi \end{aligned} \quad (4.10.13)$$

and

$$\begin{aligned} \theta_2 \Phi &= [L_{oo} + L_{oc} C(1)] \Phi \\ &= [L_{oo} + L_{oc} C(o)] \Phi = 0 \end{aligned} \quad (4.10.14)$$

etc.

These results together with eq. (6) show that

$$\Theta \bar{\Phi} = 0 \quad (4.10.15)$$

and

$$C \bar{\Phi} = C(0) \bar{\Phi} = \bar{\Phi}_c \quad (4.10.16)$$

Using eq. (16),

$$\begin{aligned} P_b \bar{\Phi} &= (P_c - C) \bar{\Phi} \\ &= \bar{\Phi}_c - \bar{\Phi}_c = 0, \end{aligned} \quad (4.10.17)$$

therefore

$$\hat{\pi} \bar{\Phi} = \bar{P}_b N_c^{-1} P_b \bar{\Phi} = 0, \quad (4.10.18)$$

which shows that  $\bar{\Phi}$  must be confined to the asymptotic subspace, i.e.

$$\tilde{\pi} \bar{\Phi} = \bar{\Phi}, \quad (4.10.19)$$

whenever  $\bar{\Phi}$  is an invariant such that  $\bar{\Phi}_c$  is regular and non-invariant.

In terms of the Laplace transform  $\Upsilon_c(z)$  of  $T_c(t)$  and  $C(z) = -i \Upsilon_c(z) L_{c0}$ , eq. (3) can be written (ref. <sup>4</sup>) p. 24) as

$$\frac{1}{z} C(z) \bar{\Phi}_0 + [\Upsilon_c(z) - \frac{1}{z}] \bar{\Phi}_c = 0 \quad (4.10.20)$$

i.e.

$$C(z) \Phi_0 + [z\gamma_c(z) - 1] \Phi_c = 0 \quad (4.10.21)$$

Using the asymptotic assumption in the form of condition (4.7.8), the assumed properties of  $\Phi_c$  imply that

$$\lim_{z \rightarrow +i0} z \gamma_c(z) \Phi_c = 0 \quad (4.10.22)$$

and ensure the existence of the expression

$$\lim_{z \rightarrow +i0} C(z) \Phi_0 = C(0) \Phi_0 = \Phi_c \quad (4.10.23)$$

Eqs. (23) follow from eqs. (6) and (21).

Now

$$\Psi_z(z) = L_{oc} \gamma_c(z) L_{co} = i L_{oc} C(z) \quad (4.10.24)$$

therefore

$$-i \Psi_z(+i0) \Phi_0 = L_{oc} C(+i0) \Phi_0 = L_{oc} C(0) \Phi_0 \quad (4.10.25)$$

and, consequently, eq. (7) may be written as

$$[L_{oo} - i \Psi_z(+i0)] \Phi = 0 \quad (4.10.26)$$

(ref. <sup>4</sup>) p. 25), and this was shown to be equivalent to eq. (8).

Now consider the case where  $\Phi_c$  has the properties

$$[L_{oo} - i\Psi_z(+i0)]\Phi = 0 \quad (4.10.27)$$

and

$$\Phi_c = C\Phi_o \quad (4.10.28)$$

From eqs. (1) and (21)

$$[L_{oo} - i\Psi_z(z)]\Phi + iz\Theta(z)\Phi_c = 0 \quad , \quad (4.10.29)$$

where  $\Theta(z) = -iL_{oc}\Upsilon_c(z)$  (ref. " ) p. 25). The proof of eq.

(29) is as follows:

From eqs. (1) and (21)

$$L_{oo}\Phi_o + L_{oc}[C(z)\Phi_o + z\Upsilon_c(z)\Phi_c] = 0 \quad , \quad (4.10.30)$$

therefore

$$[L_{oo} + L_{oc}C(z)]\Phi + zL_{oc}\Upsilon_c(z)\Phi_c = 0 \quad , \quad (4.10.31)$$

or equivalently, using eq. (24),

$$[L_{oo} - i\Psi_z(z)]\Phi + iz\Theta(z)\Phi_c = 0 \quad , \quad (4.10.32)$$

as required.

Now from condition (27) and eq. (29),

$$z\Theta(z)\Phi_c = 0 \quad , \quad (4.10.33)$$

which implies that  $\Phi_c$  is a regular supervector. In addition, using condition (28) and eqs. (4.7.17) and (4.7.23),

$$\begin{aligned}
 L \Phi &= L_{oo} \Phi_o + L_{oc} \Phi_c + L_{co} \Phi_o + L_{cc} \Phi_c \\
 &= [L_{oo} + L_{oc} C] \Phi_o + [L_{co} + L_{cc} C] \Phi_o \\
 &= \Theta \Phi_o + C \Theta \Phi_o,
 \end{aligned} \tag{4.10.34}$$

therefore, using condition (27),

$$L \Phi = 0. \tag{4.10.35}$$

The results (8), (16), (19), (33) and (35) may be summarized as follows:

For any invariant supervector  $\Phi$ , the condition that  $\Phi_c$  be regular and non-invariant is equivalent to the conditions

$$[L_{oo} - i\bar{\Psi}_2(+i0)] \Phi' = 0 \tag{4.10.36}$$

(or equivalently  $\Theta \Phi = 0$  (see eq. (26) and the subsequent statement)) and

$$\Phi_c = C \Phi_o, \tag{4.10.37}$$

which in turn imply the relation

$$\Phi = \tilde{\Pi} \Phi \quad (4.10.38)$$

Now it can be shown that the above three sets of conditions on  $\Phi$  are equivalent:

It is first shown that

$$\Phi = \tilde{\Pi} \Phi \Rightarrow \Phi_c = C \Phi_o \quad (4.10.39)$$

as follows:

The left hand equation is equivalent to

$$(P_o + C) \frac{1}{1+DC} (P_o + D) \Phi = \Phi \quad (4.10.40)$$

By equating components in the  $P_o$  and  $P_c$  subspaces, eq.

(40) gives

$$P_o \frac{1}{1+DC} (P_o + D) \Phi = \Phi_o \quad (4.10.41)$$

and

$$C \frac{1}{1+DC} (P_o + D) \Phi = \Phi_c \quad (4.10.42)$$

but eq. (41) implies that

$$C \frac{1}{1+DC} (P_o + D) \Phi = C \Phi_o \quad (4.10.43)$$

A comparison of eqs. (42) and (43) shows that  $\Phi_c = C \Phi_o$  which is the right hand equation of relation (39).

Secondly it is shown that  $\Theta \Phi = 0$  as follows:



It is given that  $L\Phi = 0$  hence that  $P_O L\Phi = 0$ , or equivalently

$$L_{oo}\Phi_O + L_{oc}\Phi_c = 0 \quad . \quad (4.10.44)$$

Using relation (39), eq. (44) gives

$$[L_{oo} + L_{oc}C]\Phi_O = 0 \quad , \quad (4.10.45)$$

or equivalently, using eq. (4.7.17),

$$\Theta\Phi_O = 0 \quad , \quad (4.10.46)$$

i.e.

$$\Theta\Phi = 0 \quad . \quad (4.10.47)$$

Together, the results (39) and (47) may be summarized as follows:

For any invariant  $\Phi$ ,  $\Phi = \tilde{\Pi}\Phi$  implies that  $\Theta\Phi = 0$  and  $\Phi_c = C\Phi_O$ .

Comparing this result with the equivalence relations involving eqs. (36), (37) and (38), the following is seen to be true:

For any invariant  $\Phi$ , the condition  $\Phi = \tilde{\Pi}\Phi$  is equivalent to the conditions that  $\Phi$  be regular and  $\Phi_c$  be non-invariant. In other words the asymptotic subspace contains all the regular invariants and only the invariants which are regular

(this result is stated in ref. <sup>4</sup>) p. 25). Singular invariants are confined to the fluctuation subspace.

#### 4.11 Condition of Dissipativity

Since homogeneous systems are of central importance in this thesis,  $L_{00}$  may be taken to be zero. Considering eq. (4.10.26) and the subsequent statement, this implies that for any supervector  $\Phi$ ,

$$\Theta \Phi = 0 \iff \Psi_{\ell} (+i0) \Phi = 0. \quad (4.11.1)$$

Consider a system for which  $\Psi_{\ell} (+i0) \equiv 0$ . From the equivalence relation (1) this implies that  $\Theta = 0$ , but since, according to eq. (4.7.14),  $\Theta$  is the infinitesimal time displacement operator in the asymptotic subspace, this implies that all supervectors in the asymptotic subspace are stationary.

The condition

$$\Psi_{\ell} (+i0) \neq 0 \quad (4.11.2)$$

is called the Condition of Dissipativity (ref. <sup>4</sup>) pp. 25, 26). The physical interpretation of this condition is given in section 4.12.

#### 4.12 Physical Interpretation of the Theory

##### Macroscopic Observations and Subdynamics

Two requirements that were imposed on the operators

representing the observables for which the theory holds are that they be regular operators and that they correspond to reduced quantities (see section 4.5 and the second last paragraph of section 4.6). Thermodynamic quantities are of this type.

The set of observables defining the macroscopic level of observation is further restricted by the consideration of time scales. A macroscopic measurement is one that takes a very long time compared with the time for microscopic processes. The interaction between the macroscopic system and the macroscopic observer (or observing device) lasts for a time interval  $T \gg \tau_c$ , where  $\tau_c$ , introduced in section 4.6, is the characteristic time for atomic processes. Quantities which decay to zero at a rate of the order of  $\tau_c$  will therefore not contribute to the results of the measurement.

These considerations show that  $\tilde{\rho}(t)$  is the only part of the density supervector that is relevant to the macroscopic description, since the expression  $\text{tr}[\hat{\rho}(t)A]$  decays to zero with a relaxation time of the order of  $\tau_c$  whenever  $A$  represents an observable of the type described in the first paragraph of this section. In setting up an initial value problem by giving  $\rho(0)$ , resulting from a macroscopic preparation of the system, it would not be possible to specify the component  $\hat{\rho}(0)$ . Because of its rapidly decaying behaviour, as described above, this would imply a specification of the origin of time,  $t = 0$ , to an accuracy of the order of  $\tau_c$ . Since a macroscopic measurement requires a time interval of duration  $T$ , this would be impossible.

The results of section 4.9, in particular the conclusions following eqs. (4.9.25) and (4.9.35), to the effect that  $\tilde{\rho}(t)$  evolves independently of  $\hat{\rho}(t)$  and in the  $\tilde{\Pi}$  subspace, orthogonal to the  $\hat{\Pi}$  subspace to which  $\hat{\rho}(t)$  is confined, makes it possible to associate the subdynamics in the  $\tilde{\Pi}$  subspace with the macroscopic level of description of the system on the basis of quantum mechanics.

The conclusion of the above considerations is that the operators  $A$  representing macroscopic observables are subject to the conditions that:

1. they are regular operators,
2. they correspond to reduced properties, and
3.  $\text{tr}(\tilde{\rho}A) \neq 0$  for an arbitrary supervector  $\tilde{\rho}$  in the  $\tilde{\Pi}$  subspace. Since the only part of  $A$  relevant to the  $\tilde{\Pi}$  subdynamics is the component  $\tilde{\Pi}A$ , this is equivalent to the condition that  $A = \tilde{\Pi}A$ .

### Non-dissipative Systems

By definition (4.11.2),  $\tilde{\Psi}_{\mathcal{L}}(+i0) \equiv 0$ , therefore, from the equivalence relation (4.11.1),  $\theta = 0$ . From eq. (4.9.15), this implies that  $\tilde{\Sigma}(t)$  is independent of time, therefore all supervectors in the  $\tilde{\Pi}$  subspace are invariant. The whole evolution of the system therefore has to be described in the  $\hat{\Pi}$  subspace in terms of microscopic observables. For such a system there is no description at the macroscopic level and all processes occur in a reversible way at the rate of atomic interactions.

The decomposition of the hamiltonian  $H = H^{(0)} + H^{(1)}$  is

equivalent to the decomposition of the Liouville superoperator  $L = L^{(0)} + L^{(1)}$  where

$$L^{(0)} = \frac{1}{\hbar} [H^{(0)}, \quad ] \quad , \quad L^{(1)} = \frac{1}{\hbar} [H^{(1)}, \quad ] \quad . \quad (4.12.1)$$

Consider the set of invariants of the system with respect to  $L^{(0)}$ . These are linear combinations of the supervectors  $|m\rangle\langle m|$  constructed from the eigenstates  $|m\rangle$  of  $H^{(0)}$ . Denote by  $B_0$  such an invariant supervector. Consider  $B = B_0 + B_c$  (where  $B_c$  is as yet undetermined). According to eqs. (4.10.36) and (4.10.37) the conditions for  $B$  to be an invariant of  $L$  are that

$$B_c = C B_0 \quad (4.12.2)$$

and

$$\Theta B = 0 \quad . \quad (4.12.3)$$

For a non-dissipative system  $\Theta = 0$  and only condition (2) remains, hence any invariant of  $L^{(0)}$  may be extended to an invariant  $B = B_0 + B_c$  of  $L$ , by defining  $B_c = C B_0$  (ref. <sup>15</sup>) pp. 791, 792). It is the existence of this class of invariants which prevents a non-dissipative system from tending to equilibrium. This is analogous to metrical decomposability of the energy surface in classical ergodic theory (ref. <sup>9</sup>) p. 265).

### Dissipative Systems

For dissipative systems  $\Psi_x(+i0) \neq 0$ , hence  $\tilde{\Sigma}(t)$  is time dependent and describes new channels of evolution in the  $\tilde{\Pi}$  subspace, which for a non-dissipative system would have been invariants of the motion. The macroscopic observables now evolve as a result of these long term processes occurring in the  $\tilde{\Pi}$  subspace.

The condition of dissipativity expresses the possibility of these long term persistent effects occurring as a result of the combined effect of the elementary processes taking place at the atomic level. It is only for such a system that there exists a macroscopic level of description, in terms of the variables of the  $\tilde{\Pi}$  subspace, of the kind discussed at the beginning of this section.

According to eq. (4.7.18)  $\tilde{\rho}_c(t)$  is a dependent variable, while  $\tilde{\rho}_o(t)$  is an independent variable. This result made it possible to derive eq. (4.7.14), an independent equation of motion for  $\tilde{\rho}_o(t)$ . The physical interpretation of this property is that a macroscopic observer has no control over the correlations. (The case of turbulent fluid motion, in which long-range correlations are produced by external macroscopic action, is not considered here.) These are produced by the interactions between the elementary constituents of the system and are continually being created and destroyed at the rate of the elementary processes (c.f. the discussion in ref. <sup>12</sup>) pp. 19, 20). This behaviour is expressed by the transitions, between states  $v, v'$  of different correlation, in eqs. (4.6.16) - (4.6.19). In agreement with the fact that it is impossible to define the initial time

$t = 0$ , at which a macroscopic measurement is made, to an accuracy of the order of  $\tau_c$ , the correlations chosen for the initial condition at time  $t = 0$  must be chosen as if they have appeared by the same mechanism as those which appear at later times (c.f. ref. <sup>12</sup>) p. 20). This is expressed by the condition  $\tilde{\rho}_c(0) = C\tilde{\rho}_0(0)$  which expresses the fact that they were created from the vacuum of correlations by the elementary collision processes. The dynamics of correlations shows therefore that any accidental correlations, produced by the intervention of an external observer, may be disregarded at the macroscopic level of description, since they are dissipated instantly (more precisely, after a time interval of the order of  $\tau_c$ ). This is expressed mathematically by the confinement of these non-dynamical correlations to the subspace  $\hat{\Pi}$  and the rapidly decaying behaviour of  $\hat{\rho}(t)$ .

The following considerations are concerned with the approach to equilibrium.

The conditions for the supervector  $B$  to be an invariant in the  $\tilde{\Pi}$  subspace are given by eqs. (2) and (3). For a dissipative system  $\theta \neq 0$  (since  $\Psi_{\pm}(+i0) \neq 0$ ) and requirement (3) is consequently a very restrictive one which can only be satisfied by a very small class of observables (ref. <sup>15</sup>) pp. 791, 792). According to the discussion involving eqs. (4.10.36) - (4.10.38), the supervector  $B$  must be regular. Now it can be shown<sup>16</sup>) that for a weakly coupled  $N$ -body system, the only regular invariants are those of the form  $f(H)$ , where  $H$  denotes the hamiltonian. It is plausible that this is true for any dissipative system. For such a system, this points to its ergodicity as follows:

Consider such a system prepared, at time  $t = 0$ , in a non-equilibrium state described by the statistical mixture  $\tilde{\rho}(0)$  such that the energy density is known to be in the interval  $(E, E+\Delta E)$ . The time evolution of  $\tilde{\rho}_0(t)$  is given by eq. (4.7.14), or equivalently by

$$\tilde{\rho}_0(t) = e^{-i\theta t} \tilde{\rho}_0(0) \quad . \quad (4.12.4)$$

The non-vanishing of  $\theta$  is not sufficient to ensure that  $\tilde{\rho}_0(t)$  is constant, but the further condition (which always seems to be true) that the supervector  $-i\theta$  be negative semi-definite, is sufficient, since the quantity

$$\chi \equiv \text{tr}(\tilde{\rho}_0^+ \tilde{\rho}_0) = \text{tr}(\tilde{\rho}_0^2) \quad (4.12.5)$$

satisfies the properties

$$\chi \geq 0 \quad (4.12.6)$$

and

$$\begin{aligned} \frac{\partial \chi}{\partial t} &= \frac{\partial}{\partial t} \text{tr}(\tilde{\rho}_0^2) = \text{tr}\left(\frac{\partial}{\partial t} \tilde{\rho}_0^2\right) \\ &= \text{tr}(2\tilde{\rho}_0 \dot{\tilde{\rho}}_0) = \text{tr}[2\tilde{\rho}_0(-i\theta)\tilde{\rho}_0] \leq 0 \quad , \end{aligned} \quad (4.12.7)$$

where the last inequality is a result of the negative semi-definiteness of  $-i\theta$ . Conditions (6) and (7) are sufficient for the result



$$e^{-i\Theta t} \tilde{\rho}_0(o) \xrightarrow{t \rightarrow \infty} \tilde{\rho}_0(\infty) \quad (4.12.8)$$

to be satisfied.

Now using relation (4.10.39),  $\tilde{\rho}_c(\infty) = C\tilde{\rho}_0(\infty)$  follows from  $\tilde{\rho}(t) = \tilde{\Pi}\tilde{\rho}(t)$ , but from the equivalence of eq. (4.10.38) and the pair of eqs. (4.10.36) and (4.10.37), it is also true that the pair of equations,  $\tilde{\rho}_c(\infty) = C\tilde{\rho}_0(\infty)$  and  $\Theta\tilde{\rho}_0(\infty) = 0$ , imply that

$$L\tilde{\rho}(\infty) = 0 \quad (4.12.9)$$

Eq. (9) shows that  $\tilde{\rho}(\infty)$  is an invariant of  $L$ . From the above considerations concerning the regular invariants,  $\tilde{\rho}(\infty)$  is assumed to be of the form  $f(H)$ . Since the energy density was found to be in the interval  $(E, E+\Delta E)$ ,  $f(H)$  will be the corresponding microcanonical ensemble. (For macroscopic observables this ensemble is equivalent to the corresponding canonical ensemble (ref. <sup>7</sup>) chapt. 5 sect. 25).)

### Summary and Further Points of Interpretation

The condition of dissipativity allows for the existence of a macroscopic description, confined to the  $\tilde{\Pi}$  subspace, in terms of  $\tilde{\rho}(t)$ . Because  $\tilde{\Pi}$  is not a projector in the strict mathematical sense ( $\tilde{\Pi}$  is not a factorizable superoperator), this description cannot be given in terms of a pure state of the form  $|\Psi\rangle\langle\Psi|$ , but only in terms of a mixture  $\tilde{\rho}(t)$ . A macroscopic observer can only describe the "state" of the system at any initial time,  $t = 0$ , as being given by a

supervector  $\tilde{\rho}(0)$ . On the basis of this information, the evolution of  $\tilde{\rho}$ , given by  $\tilde{\rho}(t) = \tilde{\Sigma}(t)\tilde{\rho}(0)$  for  $t \geq 0$ , indicates what the results of future measurements may be. For a dissipative system the behaviour of  $\tilde{\rho}(t)$  is irreversible.

On the other hand, the description of the system at the atomic level involves the entire superspace  $(\tilde{\Pi} + \hat{\Pi})$ . The initial condition may be given as a pure state, and the time evolution of this pure state may be observed. This description could just as well be given in the Hilbert space formulation. The behaviour of  $\rho(t)$  is thus reversible, but does not conflict with the irreversible behaviour of  $\tilde{\rho}(t)$ . The conditions of observation are completely different. The irreversibility of the macroscopic motion is not due to any preferred direction in time of the supervectors  $\tilde{\Pi}$  and  $\tilde{\Sigma}(t)$ . In section 4.9 these were shown to be time-reversal invariant. Equivalently,  $\tilde{\rho}(t)$  is a solution of the Liouville equation which is time-reversal invariant. For a dissipative system the irreversible behaviour comes from the fact that the initial conditions are restricted to a certain class, and that the subsequent measurements are of the same restricted type. (The symmetry in time of  $\tilde{\Sigma}(t)$  does lead one to the conclusion that the retrodiction one makes on the state of the system, on the basis of the knowledge of  $\tilde{\rho}(0)$ , is the same as the prediction one makes on the basis of the same information. In other words  $\tilde{\rho}(-t) = \tilde{\rho}(t)$ .)

The argument was put forward that an invariant is regular if and only if it is a function of  $H$ . If this is true, then all invariants in the  $\tilde{\Pi}$  subspace are functions of  $H$ . Hence

for the macroscopic description, all the other invariants (the singular invariants which are confined to the  $\hat{\Pi}$  subspace) may be ignored. They do not prevent the approach to equilibrium of  $\tilde{\rho}(t)$ . According to the argument following eq. (9),  $\tilde{\rho}(\infty)$  depends only on the interval of energy  $(E, E+\Delta E)$  and not on any further specifications of  $\tilde{\rho}(0)$ .

## 5. RESOLUTION OF THE MEASUREMENT PROBLEM

### BY THE APPROACH OF THE BELGIAN GROUP

Denote by I the system, of atomic dimensions, to be observed and let the observable of interest be represented by the hermitian operator  $A$ . Denote by II the system, of macroscopic dimensions, which serves as the apparatus, and choose the origin of time as the time instant at which the measurement interaction occurs.

In order to serve as the measuring apparatus, system II has to have certain characteristics. The Hilbert space of system II has a complete orthogonal basis  $\{|k m\rangle\}_{k m}$  with the following specifications (c.f. ref. <sup>4</sup>) p. 36):

1. The correlations between states  $|k m\rangle$  with common index  $k$  is very much stronger than the correlations between states with different indices  $k$ . The latter correlations must be sufficiently weak so that to each manifold  $k$  there corresponds a transient macrostate of sufficient duration to be observed, or registered directly by macroscopic means. If the apparatus is to register a permanent record, each manifold  $k$  will be invariant.

2. Before the measurement interaction the apparatus will be in the equilibrium "state" of some manifold  $k = 0$ . This manifold must be effectively invariant at least for a time interval longer than the duration of the experiment. At this stage  $\rho^{II}$  will be given as the equilibrium ensemble for that manifold. The manifold  $k = 0$  is a subspace of the energy shell corresponding to a given energy interval  $(E, E + \Delta E)$ , as

is the case in the ergodic approach.

3. Without loss of generality, it is assumed, for convenience of notation, that the spectrum of  $A$  is discrete and non-degenerate (recall the discussion following eq. (3.2.6)). Let  $A|\phi_k\rangle = a_k|\phi_k\rangle$  and let the initial state of system I be given by

$$|\phi(0)\rangle = \sum_k c_k |\phi_k\rangle \quad (5.1)$$

During the measurement interaction, of atomic duration  $\tau$  at time  $t = 0$ , between systems I and II, each eigenstate  $|\phi_k\rangle$  causes the manifold  $k$  to be occupied with a probability equal to  $|c_k|^2$ .

The discussion of the duration and strength of the interaction, compared with the hamiltonians of systems I and II, is the same as that given in section 3.2. The interaction conserves the coarse-grained energy, given by the interval  $(E, E+\Delta E)$ , of system II, hence the manifolds  $k$  that may be occupied all correspond to the same energy shell.

Following the terminology of section 2.1, the manifolds  $k$  are henceforth referred to as channels.

With the above specifications of system II, the measurement process may be described as follows:

Let  $H_I$ ,  $H_{II}$  and  $H_{INT}$  denote the hamiltonians of systems I and II and the interaction between I and II respectively. Define the Liouville superoperators

$$L_I = \frac{1}{\hbar} [H_I, ] \quad L_{II} = \frac{1}{\hbar} [H_{II}, ] \quad L_{INT} = \frac{1}{\hbar} [H_{INT}, ] \quad (5.2)$$

Let  $|\phi_0\rangle$  denote any state vector of system II in channel  $k = 0$ . As in the ergodic approach, the interaction at time  $t = 0$  between systems I and II has the following effect:

$$e^{-\frac{i}{\hbar}(H_I + H_{II} + H_{INT})\tau} \left( \sum_k c_k |\phi_k\rangle |\Phi_0\rangle \right) = \sum_k c_k e^{-\frac{i}{\hbar}H_I\tau} |\phi_k\rangle e^{-\frac{i}{\hbar}H_{II}\tau} |\Phi_k\rangle$$

$$\approx \sum_k c_k |\phi_k\rangle |\Phi_k\rangle, \quad (5.3)$$

taking  $\tau \approx 0$ . In the superspace notation this is written as

$$e^{-i(L_I + L_{II} + L_{INT})\tau} \left( \sum_{kk'} c_k c_{k'}^* |\phi_k\rangle \langle \phi_{k'}| \cdot |\Phi_0\rangle \langle \Phi_0| \right)$$

$$\approx \sum_{kk'} c_k c_{k'}^* |\phi_k\rangle \langle \phi_{k'}| \cdot |\Phi_k\rangle \langle \Phi_{k'}|. \quad (5.4)$$

The following projection superoperators, defined on the superspace of system II, will be required:

$$P^{kk'} = \sum_{mm'} [ |k m\rangle \langle k m| \times |k' m'\rangle \langle k' m'| ] \quad (5.5)$$

$$P_0 = \sum_{km} [ |k m\rangle \langle k m| \times |k m\rangle \langle k m| ] \quad (5.6)$$

$$P_c = I - P_0, \quad (5.7)$$

where, in the limit of an infinite system, any summation is to be understood as an integration. The projection  $P^{kk'}_{\rho}^{II}$

is denoted by  $\rho_{kk'}^{II}$ .

Consider a statistical mixture  $\rho_{00}^{II}$  of states of the form  $|\Phi_0\rangle$ . From eq. (4) the interaction between systems I and II has the following effect:

$$|\phi_k\rangle\langle\phi_{k'}| \cdot |\Phi_0\rangle\langle\Phi_0| \rightarrow |\phi_k\rangle\langle\phi_{k'}| \cdot |\Phi_k\rangle\langle\Phi_{k'}| \quad , \quad (5.8)$$

hence for the supervector  $\rho_{00}^{II}$ , making use of the linearity of the evolution superoperator for the composite system,

$$|\phi_k\rangle\langle\phi_{k'}| \rho_{00}^{II} \rightarrow |\phi_k\rangle\langle\phi_{k'}| \rho_{kk'}^{II} \quad . \quad (5.9)$$

From eq. (9) and the linearity of the evolution superoperator, the interaction between systems I and II, for the case in which system II is initially in the state represented by the density supervector  $\rho_{00}^{II}$ , is represented by

$$e^{-i(L_I + L_{II} + L_{int})\tau} \sum_{kk'} c_k c_{k'}^* |\phi_k\rangle\langle\phi_{k'}| \rho_{00}^{II} = \sum_{kk'} c_k c_{k'}^* |\phi_k\rangle\langle\phi_{k'}| \rho_{kk'}^{II} \quad (5.10)$$

taking  $\tau \approx 0$ .

According to condition 2,  $\rho_{00}^{II}$  is the equilibrium distribution for the channel  $k = 0$ . On the other hand  $\rho_{kk}^{II}$  for  $k \neq 0$  will be a non-equilibrium distribution for channel  $k$ .

After the measurement interaction systems I and II evolve independently of one another according to their respective Liouville superoperators  $L_I$  and  $L_{II}$ . Therefore the density supervector for the combined system at any time  $t > 0$  is given, using eq. (10), as

$$\rho^{I+II}(t) = \sum_{kk'} c_k c_{k'}^* e^{-iL_I t} |\phi_k\rangle \langle \phi_{k'}| e^{-iL_{II} t} \rho_{kk'}^{II}. \quad (5.11)$$

Since system II is to be treated as a macroscopic system, the terms

$$\rho_{kk'}^{II}(t) = e^{-iL_{II} t} \rho_{kk'}^{II} \quad (5.12)$$

occurring in the R.H.S. of eq. (11) must be replaced by  $\tilde{\Sigma}(t) \rho_{kk'}^{II}$ , where  $\tilde{\Sigma}(t)$  defined by eq. (4.9.15) denotes the asymptotic evolution superoperator for system II.

The evolution of the components  $\rho_{kk'}^{II}$ , for  $k \neq k'$  is very important in this discussion. It appears as a factor in the term  $c_k c_{k'}^* |\phi_k\rangle \langle \phi_{k'}| \cdot \rho_{kk'}^{II}$ , which, since it has  $c_k c_{k'}^*$ , as a factor, exhibits the contribution to the density supervector for the combined system due to the phase relations, which existed before the interaction, between the states  $|\phi_k\rangle$  and  $|\phi_{k'}\rangle$ . These components must be shown to have no effect on observations on the combined system whenever system II is observed as a macroscopic system. This is shown to be the case in the following way:

First it is necessary to make a further assumption.

4. The supervector  $\rho_{kk'}^{II}$  is regular for each pair  $(k, k')$ . This assumes that the interaction between systems I and II does not introduce any extraneous ordering of the elementary constituents of system II.

Using condition 1 it is possible to make the approximation

$$L_{oc} \rho_{kk'}^{II} = 0, \quad (5.13)$$



where  $L$  is to be understood as referring to  $L_{II}$ . Since by definition of  $P_0$  and  $P_c$ ,  $P_0 \rho_{kk'}^{II} = 0$  for  $k \neq k'$ , it follows that for  $k \neq k'$ ,

$$L_{00} \rho_{kk'}^{II} = 0, \quad L_{c0} \rho_{kk'}^{II} = 0. \quad (5.14)$$

Eqs. (13) and (14) imply that for  $k \neq k'$ ,

$$L \rho_{kk'}^{II} = L_{cc} \rho_{kk'}^{II}, \quad (5.15)$$

therefore, for  $k \neq k'$ ,

$$e^{-iLt} \rho_{kk'}^{II} = e^{-iL_{cc}t} \rho_{kk'}^{II}. \quad (5.16)$$

Eq. (16), together with assumption 4 and the asymptotic hypothesis (4.7.7), shows that for  $k \neq k'$  the expression  $\rho_{kk'}^{II}(t)$  decays to zero on the atomic time scale. In terms of the decomposition of the superspace of system II by means of the projectors  $\tilde{\Pi}$  and  $\hat{\Pi}$ , this result is expressed by

$$\tilde{\Pi} e^{-iLt} \rho_{kk'}^{II} = 0 \quad (k \neq k'), \quad (5.17)$$

or equivalently, from eq. (4.9.25), by

$$\tilde{\Sigma}(t) \rho_{kk'}^{II} = 0 \quad (k \neq k'). \quad (5.18)$$

This shows that, for  $k \neq k'$ ,  $\rho_{kk'}^{II}$  is a supervector in the fluctuation subspace of system II.

It now remains to study the expressions of the form  $e^{-iL_{II}t} \rho_{kk}^{II}$  which appear in eq. (11).

In order to make clear the equivalence of this approach to the measurement problem with that of the Italian group, the hamiltonian  $H_{II}$  is written as

$$H_{II} = \sum_k H^k + \sum_{k \neq k'} H^{kk'} \quad , \quad (5.19)$$

where  $H^k = p^{kk} H_{II}$ ,  $H^{kk'} = p^{kk'} H_{II}$  ( $k \neq k'$ ) and, by virtue of condition 1,  $H^{kk'} \approx 0$ . (For convenience of notation the subscript II is occasionally dropped.)

In order that system II tends to equilibrium in each channel  $k$ , it is necessary to have a condition of dissipativity on the evolution of system II in each channel  $k$ . This condition is stated as

$$5. \quad \Psi_{II}^k(+i0) \neq 0 \quad , \quad (5.20)$$

where

$$\Psi_{II}^k(z) = -iz L_{oc}^k \frac{1}{L_{cc}^k - z} L_{co}^k \quad (5.21)$$

and

$$L^k = \frac{1}{\hbar} [H^k, \quad] \quad (5.22)$$

According to the discussion in section 4.12 on the regular invariants of dissipative systems, and on the basis of condition 5 (eq. (20)), the only regular invariants of  $L^k$  are

functions of  $H^k$ . Considering the evolution of  $\rho_{kk}^{II}$  at the macroscopic level, the discussion in section 4.12 on the approach to equilibrium shows that

$$\tilde{\Sigma}(t) \rho_{kk}^{II} \xrightarrow[t \rightarrow \infty]{} f(H^k) , \quad (5.23)$$

where  $f(H^k)$  is the microcanonical ensemble (or equivalently the canonical ensemble) corresponding to the energy interval  $(E, E+\Delta E)$  introduced in condition 2.

Returning to eq. (11) and using the results (18) and (23), the density supervector for the composite system, where system II is observed as a macroscopic system, becomes

$$\begin{aligned} \rho^{I+II}(t) &= \sum_{kk'} c_k c_{k'}^* e^{-iL_I t} |\phi_k\rangle \langle \phi_{k'}| \tilde{\Sigma}(t) \rho_{kk}^{II} \delta_{kk'} \quad \forall t > 0 \\ &= \sum_k |c_k|^2 e^{-iL_I t} |\phi_k\rangle \langle \phi_k| \tilde{\Sigma}(t) \rho_{kk}^{II} \quad \forall t > 0 \end{aligned} \quad (5.24)$$

$$\xrightarrow[t \rightarrow \infty]{} \sum_k |c_k|^2 e^{-iL_I t} |\phi_k\rangle \langle \phi_k| f(H^k) . \quad (5.25)$$

Eq. (24) expresses the result that all trace of the coefficients  $c_k c_{k'}^*$ , for  $k \neq k'$  has been eliminated. Statement (25) expresses the fact that in each channel  $k$ , the apparatus tends towards a unique equilibrium state, and once system II has reached equilibrium, the state of the composite system is described by a statistical mixture of states  $k$ , each of which corresponds to system I being in a particular state

$$|\phi_k(t)\rangle = e^{-\frac{i}{\hbar} H_I t} |\phi_k\rangle \quad (5.26)$$

with the apparatus in the unique equilibrium macrostate defined by the supervector  $f(H^k)$ . In addition, the statistical weight of state  $k$  is  $|c_k|^2$  and this is independent of any reference to the apparatus (system II).

It is possible to obtain a formal expression referring only to system I, as was done in the ergodic approach, resulting in eq. (3.2.22). From eq. (24), writing

$$e^{-iL_I t} = e^{-\frac{i}{\hbar} H_I t} \times e^{\frac{i}{\hbar} H_I t}, \quad (5.27)$$

one obtains

$$\rho^I(t) = \sum_k |c_k|^2 e^{-\frac{i}{\hbar} H_I t} |\phi_k\rangle \langle \phi_k| e^{\frac{i}{\hbar} H_I t}. \quad (5.28)$$

This is precisely the result required by the measurement algorithm of quantum mechanics.

Two points which must be stressed for the sake of the comparison with the ergodic approach are:

1. The demonstration of the vanishing of the phase relations between the eigenstates  $|\phi_k\rangle$  of the atomic system (system I) was made possible through the asymptotic hypothesis. This was done in the derivation of eq. (18).
2. The formation of a permanent record of the result of the measurement by the apparatus (system II) required a condition of dissipativity to be obeyed in each channel  $k$ .

## 6. MODIFIED MACROSCOPIC DESCRIPTION

The macroscopic description involving the  $\tilde{\Pi}$  subspace may be formulated in an alternative way which is exactly equivalent, since it arises as a result of certain exact properties of the evolution in the  $\tilde{\Pi}$  subspace and of the properties of the superoperator  $\tilde{\Pi}$ . The modified description, given in this section, makes it easier to show how the macroscopic description involving the  $\tilde{\Pi}$  subspace is consistent with the formal reduction rule of quantum mechanics, and to formulate the comparison with the ergodic approach.

The macroscopic description cannot be formulated in terms of eigenstates and operators as is done in the description of an atomic system. If the result of the measurement of the observable  $A$  at time  $t = 0$  is to show that  $A$  is in the interval  $(a, a+da)$ ,  $\rho(0)$  is not to be constructed on the basis of equal a priori probabilities and random phases as a mixture of eigenstates, of the operator  $A$ , with eigenvalues in the range  $(a, a+da)$ . This is due to the dissipativity of the system. On the basis of such a measurement, the state of the system is described instead by a density supervector  $\tilde{\rho}(0)$ , the structure of which is determined by the projector  $\tilde{\Pi}$  as well as by the results of the measurement. This is explained in more detail later on in this section.

The evolution of  $\tilde{\rho}(t)$  is given by the Liouville equation, and for any macroscopic observable  $B$

$$\langle B \rangle_t = \text{tr} [B \tilde{\rho}(t)] \quad . \quad (6.1)$$

Both  $\tilde{\rho}_0(t)$  and  $\tilde{\rho}_c(t)$  are relevant to  $\langle B \rangle_t$ , but because the evolution of  $\tilde{\rho}(t)$  can also be given by eqs. (4.7.14) and (4.7.19), the macroscopic description may be given in terms of  $\tilde{\rho}_0$  alone. Using eq. (4.7.19) and the transposition property of projection superoperators given by definition 6 in section 4.3,

$$\begin{aligned}
 \langle B \rangle_t &= \text{tr}[B^+ \tilde{\rho}(t)] = \text{tr}[B^+ (\tilde{\rho}_0(t) + \tilde{\rho}_c(t))] \\
 &= \text{tr}[B^+ (P_0 + C) \tilde{\rho}_0(t)] = \text{tr}[B^+ P_a \tilde{\rho}_0(t)] \\
 &= \text{tr}[(B P_a)^+ \tilde{\rho}_0(t)] \quad . \quad (6.2)
 \end{aligned}$$

Now  $B P_a$  is self-adjoint since

$$\begin{aligned}
 (B P_a)^+ &= P_a^\dagger B^+ = (P_a^\dagger B^+)^+ \\
 &= (B^+)^+ (P_a^\dagger)^\dagger = B P_a \quad (6.3)
 \end{aligned}$$

where the second equality on the first line uses the adjoint-symmetry of  $P_a^\dagger$  which follows from the adjoint-symmetry of  $P_a$ . The supervector  $B P_a$  has replaced the supervector  $B$  as the macroscopic observable.

The macroscopic description may therefore be given in terms of  $\tilde{\rho}_0$  alone which describes a probability distribution over the states  $|m\rangle$ . This distribution evolves according to the Markovian equation  $i\dot{\tilde{\rho}}_0 = \theta \tilde{\rho}_0$  (eq. (4.7.14)), which describes the evolution of this distribution without reference to phase relations at all. This implies that no quantal

interference effects occur at the macroscopic level, except for the quantum statistical effects which are incorporated in the construction of the basis states  $|m\rangle$ . Furthermore it can be seen from the structure of  $P_a$  that the modified macroscopic observables  $BP_a$  are diagonal in the representation corresponding to the basis  $\{|m\rangle\}$ . The supervectors  $BP_a$ , which appear as the macroscopic observables in this modified description, therefore commute with each other, as is required for them to be simultaneously measurable.

In this description, a complete macroscopic determination of the state of the system, at an arbitrary initial time  $t = 0$ , involves an observation of the complete set  $\{B\}$  of macroscopic observables, represented here by the set  $\{BP_a\}$  of commuting operators. (The macroscopic observables form a complete set in the sense that a self contained description in terms of them is possible.) Such an observation determines  $\tilde{\rho}_0(0)$  as follows:

Let  $|m_i\rangle$  be a simultaneous eigenstate of the operators  $\{BP_a\}$ . The supervector  $|m_i\rangle\langle m_i|$  represents a dynamical state of the system which is consistent with the specification of the system given by the results of the macroscopic measurement, but undergoes rapid changes on the atomic time scale as a result of the elementary collision processes. The asymptotic form of  $|m_i\rangle\langle m_i|$ , after a time interval of the order of several collision times  $\tau_c$ , is given by the supervector  $\tilde{\rho}^i(0) = \tilde{\Pi}|m_i\rangle\langle m_i|$ . The component  $\tilde{\rho}_0^i(0) = P_0\tilde{\rho}^i(0)$  gives a diagonal distribution over the basis states  $|m\rangle$  compatible with the measured values of the observables  $BP_a$ .

For the macroscopic description in terms of the  $\tilde{\Pi}$

subspace to have any meaning at all, it must be true that the statistical fluctuation of each observable  $BP_a$  is negligible in the state  $\tilde{\rho}_0^1(o)$ . Hence  $\tilde{\rho}_0^1(o)$ , defined above, gives the required initial state.

According to the measurement axiom of quantum mechanics, a measurement, at time  $t = 0$ , of the macroscopic observables  $\{BP_a\}$ , which are diagonal in the representation corresponding to the basis  $\{|m\rangle\}$ , results in the off-diagonal matrix elements of  $\tilde{\rho}(t)$  (in that representation) being equated to zero. Since these matrix elements are not explicitly included in the modified picture, which is entirely in terms of  $\tilde{\rho}_0$ , the formal reduction rule brings about no change in the macroscopic state of the system. The macroscopic description has thus been shown to be consistent with the reduction rule of quantum mechanics.

This can be interpreted physically as follows:

The formal elimination, in the reduction rule, of the phase relations between the basis states  $|m\rangle$  takes into account the uncontrollable perturbation in the system, at the atomic level, caused by the measuring process and resulting in the randomization of the "correlations". However, prior to the measurement, no assumption about the correlations was made other than the fact that they were created by "collisions" (recall the discussion on dissipative systems in section 4.12). The dynamics of correlations shows how the correlations are continually being created and destroyed at the rate of atomic processes. The correlations given by the supervector  $\tilde{\rho}_C(t)$  are dissipated at the rate of the order of  $\tau_C$ , but are



continually being replaced by fresh ones at the same rate, this time scale being so short compared with macroscopic times that it is regarded as instantaneous. This process is expressed by the equation  $\tilde{\rho}_c(t) = C\tilde{\rho}_0(t)$  (eq. (4.7.19)).

The perturbation produced by the measuring process disturbs the correlations during the time interval  $T$  (ideally  $\tau_c \ll T < t_R$ , where  $t_R$  is a characteristic macroscopic time interval) needed for the measurement, by introducing "non-dynamical" correlations represented in the theory by the supervector  $\hat{\rho}_c(t)$ . As discussed in section 4.12, the theory shows how all correlations are continually dissipated on the atomic time scale, but only the "dynamical" correlations are continually being restored. The accidental (non-dynamical) correlations do not persist longer than a few elementary collision times. Thus, in the macroscopic description, the measuring process does not affect the dynamical correlations which are always given by eq. (4.7.19). This is why it is possible, in the modified macroscopic description, to exclude them from the "state vector"  $\tilde{\rho}_0$  and to incorporate them in the observables  $BP_a$ .

The purpose of introducing the modified macroscopic description is to facilitate the discussion of the measuring process and the comparison with the ergodic approach. On the other hand, the description in terms of the  $\tilde{\Pi}$  subspace is convenient for discussing the invariants of the system, since the equation of motion for  $\tilde{\rho}$  is the same as that for the complete density supervector  $\rho$ , hence the set of invariants of  $L$  provides the complete set of invariants for the

microscopic description as well as the complete set of possible invariants for the macroscopic description. A new equation of motion for  $\tilde{\rho}$  might introduce a new class of invariants.

## 7. COMPARISON BETWEEN THE ERGODIC AND SUPERSPACE THEORIES

### 7.1 Macroscopic Description

For the purpose of this comparison a modified form of the  $\tilde{\Pi}$  subspace description of the macroscopic level of quantum mechanics was introduced in section 6. In this modified formalism the supervector for the macroscopic description is  $\tilde{\rho}_0$ , while the observables are the supervectors  $BP_a$  for certain supervectors  $B$  discussed in section 4.12. Also for the purpose of this comparison a coarse-graining superoperator  $C$  was defined by eq. (2.1.4).

Recall from section 6 that for any supervector  $\rho$ , the component  $\tilde{\rho}_0 = P_0 \tilde{\Pi} \rho$  gives a type of coarse-grained probability distribution over the states  $|m\rangle$ . In conjunction with the supervectors  $BP_a$ , where the supervectors  $B$  satisfy the conditions 1, 2 and 3 in the section on macroscopic observables in section 4.12,  $\tilde{\rho}_0(t)$  gives the macroscopic state of the system at time  $t$  through the relation

$$\langle B \rangle_{\tilde{\rho}(t)} = \langle BP_a \rangle_{\tilde{\rho}_0(t)} = \text{tr}[(BP_a)^+ \tilde{\rho}_0(t)] \quad (7.1.1)$$

This compares directly with the corresponding expression

$$\langle CB \rangle_{C\rho(t)} = \text{tr}[(CB)^+ (C\rho(t))] \quad (7.1.2)$$

in the ergodic approach (c.f. eq. (2.2.17)).

Thus the macroscopic state of the system at time  $t$  may be given by  $\tilde{\rho}_0(t)$ , or equivalently by  $C\rho(t)$ , and the

macroscopic observables are the supervectors  $BP_a$ , or equivalently the operators  $CB$ .

Since  $\tilde{\rho}_0$  and the observables  $BP_a$  are diagonal in the representation corresponding to the basis  $\{|m\rangle\}$ , and since  $C\rho$  and the observables  $CA$  are diagonal in the basis  $\{|akvi\rangle\}$ , the two bases play equivalent roles in the two theories.

The superspace approach shows how the macroscopic description arises partly from the dynamics of the system. However, because of the condition that all supervectors  $B$ , corresponding to macroscopic observables, are subject to conditions 1 and 2 in section 4.12, and because of the essential requirement that any macroscopic observable has a negligible dispersion in the equilibrium state  $\tilde{\rho}(\infty)$ , it is clear that coarse-graining is to a large extent implicit in the superspace theory.

## 7.2 Discussion of the Measuring Process on an Atomic System

In the ergodic approach to the measurement problem eq. (3.2.10) gives the state of the composite system of atomic system I and apparatus II at time  $t$  after the measurement interaction. This equation can be rewritten as

$$|\Psi(t)\rangle = \sum_k c_k e^{-\frac{i}{\hbar} H_I t} |\phi_k\rangle e^{-\frac{i}{\hbar} H_{II} t} |\Phi_k\rangle \quad (7.2)$$

where  $|\phi_k\rangle$  is any state in the channel  $C_k$ . In density operator notation eq. (1) was expressed equivalently by eq. (3.2.17) as

$$\rho^{I+II}(t) = |\Psi(t)\rangle\langle\Psi(t)|$$

$$= \sum_{\kappa\kappa'} c_{\kappa} c_{\kappa'}^* e^{-\frac{i}{\hbar} H_I t} |\phi_{\kappa}\rangle\langle\phi_{\kappa'}| e^{\frac{i}{\hbar} H_I t} e^{-\frac{i}{\hbar} H_{II} t} |\Phi_{\kappa}\rangle\langle\Phi_{\kappa'}| e^{\frac{i}{\hbar} H_{II} t}, \quad (7.2.2)$$

or by defining

$$L_I = \frac{1}{\hbar} [H_I, ] \quad , \quad L_{II} = \frac{1}{\hbar} [H_{II}, ] \quad , \quad (7.2.3)$$

eq. (2) can be written as

$$\rho^{I+II}(t) = \sum_{\kappa\kappa'} c_{\kappa} c_{\kappa'}^* e^{-iL_I t} |\phi_{\kappa}\rangle\langle\phi_{\kappa'}| e^{-iL_{II} t} |\Phi_{\kappa}\rangle\langle\Phi_{\kappa'}| \quad (7.2.4)$$

Consider the factor

$$\rho_{\kappa\kappa'}^{II}(t) = e^{-iL_{II} t} |\phi_{\kappa}\rangle\langle\phi_{\kappa'}| \quad (\kappa \neq \kappa') \quad (7.2.5)$$

appearing in eq. (4). The only part of this factor that is relevant to a macroscopic measurement, performed on the

apparatus at time  $t$ , is the coarse-grained part  $C\rho_{\kappa\kappa'}^{II}(t)$ .

For  $\kappa \neq \kappa'$  this is equal to zero, since the matrix elements of

$\rho_{\kappa\kappa'}^{II}(0)$  link invariant channels, which implies that  $\rho_{\kappa\kappa'}^{II}(t)$  is

also off-diagonal for all times  $t$ . Since in eq. (4), or

equivalently eq. (2), the operator  $\rho_{\kappa\kappa'}^{II}(t)$  is multiplied by

the factor  $c_{\kappa} c_{\kappa'}^*$ , which describes the phase relations between

the eigenstates  $|\phi_{\kappa}\rangle$  and  $|\phi_{\kappa'}\rangle$  of the atomic system at time

$t = 0$ , this results in the elimination of these phase

relations, as discussed in the paragraph following eq. (3.2.17).

The corresponding situation in the superspace approach is

repeated below. It was shown in section 5 that  $\rho_{kk'}^{II}$ , for  $k \neq k'$ , is a supervector in the  $\hat{\Pi}$  subspace of the superspace of system II (recall eq. (5.17)), and hence is rejected from the description of the composite system I + II in which system II is to be treated as a macroscopic system.

Naturally this is stronger than the corresponding statement in the ergodic approach, which deals only with the final equilibrium state of the apparatus. According to the superspace approach, any term  $k \neq k'$  in the sum in eq. (5.11) decays to zero on the time scale  $\tau_c$ , the atomic time scale of the apparatus, and hence is irrelevant to the description of the composite system on the macroscopic time scale even before the apparatus has reached equilibrium.

It may appear that the terms involving the factors  $c_k c_{k'}^*$ , for  $k \neq k'$ , have been eliminated without the need for the criterion of ergodicity in the ergodic approach, or dissipativity in the superspace approach. This is however not the case, since without ergodicity the macroscopic description, in terms of the cell subdivision, would be meaningless, while in the superspace approach, there would be no macroscopic level of description in terms of the  $\tilde{\Pi}$  subspace. This was discussed at the end of section 3.2 and at the end of section 5 respectively.

For the more general situation in which the channels  $C_k$  are not strictly invariant, for example in the case of the spark chamber, the results of the superspace approach, regarding the decay of the supervectors  $\rho_{kk'}^{II}(t)$ , for  $k \neq k'$ , still applies, but statement (5.23), regarding the approach to equilibrium in each channel  $k$ , now applies only for times

$t$  of the order of the relaxation time  $t_R$  (associated with the channel in question) and less than the decay time of the transient macrostate corresponding to that channel.

In the ergodic approach to this situation (recall the end of section 3.2), in order to show that the terms  $k \neq k'$  vanish, it was necessary to introduce the ergodicity condition (3.2.23). As discussed at the end of section 3.2, this ergodicity condition shows more explicitly that the vanishing of the terms  $k \neq k'$  is of ergodic nature, and compares more closely with the corresponding explanation given in the superspace approach. This situation is not discussed further, and the channels are assumed to be invariant.

It was shown that the conditions of ergodicity or dissipativity are essential for the apparatus to approach equilibrium in each channel, and hence to register the result of the measurement with a signal of a macroscopic kind. This is in any case an essential part of the measuring process, for without it system II would not be a measuring apparatus.

### 7.3 Approach to Equilibrium

According to the ergodicity conditions (2.2.8) and (2.2.9), any state vector  $\phi(o)$  in a particular channel  $C_k$ , in a given energy shell, evolves in such a way that the time average of the norm of its projection onto any cell  $C_{k_v}$  is proportional to  $S_{k_v}$ , the dimension of that cell. The system is not ergodic in the strict sense that in the course of time

the state vector  $\Phi(t)$  passes arbitrarily close to every possible state vector in that channel. This would require the condition, analogous to the condition of metrical indecomposability in classical ergodic theory, that each channel  $C_k$  cannot be decomposed into orthogonal, invariant subspaces. Instead, the Italian approach considers ergodic observables defined in terms of the cells  $C_{kv}$ . In this approach the ergodicity conditions require a type of extended condition of metrical indecomposability, in the sense that each channel  $C_k$  cannot be decomposed into orthogonal invariant subspaces such that any cell is a subspace of one of these invariant subspaces. This allows the state vector  $\Phi(t)$  to visit each cell, in spite of the existence of microscopic invariants of the motion.

In the Belgian approach the situation is similar. Here it is known that there exist singular invariants of the motion, but these do not prevent the approach to equilibrium of the macroscopic state, provided there are no regular invariants besides the hamiltonian  $H^k$  corresponding to the channel in question.

Ergodicity condition (2.2.9) states that the initial correlations in the system do not contribute to the macroscopic description (at equilibrium) in terms of the time average of the occupation probability of a particular cell  $C_{kv}$ . This is equivalent to the result in the Belgian approach that the supervector  $\hat{p}(0)$  is irrelevant to the macroscopic level of description.

According to eq. (2.2.12), obtained from ergodicity



conditions (2.2.8) and (2.2.9),

$$M u_{\kappa\nu}(t) = \frac{S_{\kappa\nu}}{S_{\kappa}} \quad . \quad (7.3.1)$$

According to this result, the equilibrium macrostate in channel  $C_k$  is the microcanonical ensemble corresponding to that channel (referred to in ref. <sup>17</sup>) as the polymicrocanonical ensemble).

This is equivalent to the statement (eq. (5.23)), in the Belgian approach, that

$$\tilde{\Sigma}(t) \rho_{\kappa\kappa}^{\pi} \xrightarrow[t]{\infty} f(H^{\kappa}) \quad , \quad (7.3.2)$$

where  $f(H^k)$  may be taken to be the microcanonical ensemble or the canonical ensemble for channel  $k$ , since, in the limit of an infinite system, these ensembles are equivalent for reduced quantities.

According to eqs. (2.2.10),

$$\frac{S_{\kappa\nu}}{S_{\kappa}} \approx \delta_{\nu e_{\kappa}} \quad . \quad (7.3.3)$$

This expresses the condition that the macroscopic observables have a vanishingly small dispersion with respect to the microcanonical ensemble for the channel  $C_k$ . This condition is also assumed to be true in the Belgian approach (sect. 4.5), as it is believed to be satisfied by reduced properties.

#### 7.4 Concluding Remarks

In section 2.2 of the Italian approach, it was stressed that the results of the theory, concerning the irreversible behaviour of the apparatus, apply asymptotically (in the sense of the limit of an infinite system). This point is also implied in the Belgian approach, since it is only in the limit of an infinite system that the component  $\rho'_0(t)$ , given by eq. (4.6.18), shows exponentially decaying behaviour in time, instead of periodic behaviour. The asymptotic hypothesis (condition (4.7.7)) therefore only applies to the limit of an infinite system.

In both theories, therefore, the reduction of the state vector of an atomic system is a process which occurs as a result of the irreversible behaviour of the apparatus, after the measurement interaction, and its approach to equilibrium, which is a process of asymptotic character.

According to these two theories, the reduction of the state vector of the atomic system is an asymptotic phenomenon, which does not conflict with the time-independent Schrödinger equation.

If the description of a large system in terms of the macroscopic observables is to have any meaning at all, it is essential that this mode of description is sufficient to describe any possible macroscopic interaction between this system and any other large system. In the Belgian approach it is to be understood that a macroscopic observer can only interact with the component  $\tilde{\rho}$  of the density supervector  $\rho$  of the system (ref. 4) sect. 4). Only under special (and

impossible) experimental conditions can he observe the behaviour of the entire system at the atomic level, given by the complete density supervector  $\rho$ . In this case the description in terms of  $\tilde{\rho}$  would not apply. This was discussed in the summary of section 4.12. In the Italian approach the macroscopic observables are to be understood as having the same significance (ref. <sup>3</sup>) sect. 11).

Since in both theories the apparatus is treated as such a macroscopic system, the measurement process performed by the apparatus on the atomic system is objectively defined, without the need for a human observer to be involved.

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